Discrete geometry approach to structure-preserving discretization of Port-Hamiltonian systems

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For those who care about structure

Abstract

This thesis addresses the issue of structure-preserving discretization of open distributed-parameter systems with generalized Hamiltonian dynamics. Employing the formalism of discrete exterior calculus, I introduce simplicial Dirac structures as discrete analogues of the Stokes-Dirac structure and demonstrate that they provide a natural framework for deriving finite-dimensional port-Hamiltonian systems that emulate their infinite-dimensional counterparts. The spatial domain, in the continuous theory represented by a finite-dimensional smooth manifold with boundary, is replaced by a homological manifold-like simplicial complex and its circumcentric dual. The smooth differential forms, in the discrete setting, are mirrored by cochains on the primal and dual complexes, while the discrete exterior derivative is defined to be the coboundary operator. This approach of discrete exterior geometry, rather than discretizing the partial differential equations, allows to first discretize the underlying Stokes-Dirac structure and then to impose the corresponding finite-dimensional port-Hamiltonian dynamics. In this manner, a number of important intrinsically topological and geometrical properties of the system are preserved. I demonstrate general considerations on a number of physical examples, including reaction-diffusion systems, where the structure-preserving discretization recovers the standard compartmental model. Furthermore, I show how a Poisson symmetry reduction of Dirac structures associated with infinite- and finite-dimensional models can be conducted in a unified fashion.

Contents

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I have no phrases to sing my family's praises.

[1]Most of the work reported in this document has been carried out in the comfort of my studio gracefully infused with the scent of dark roast, fine wine, and the best fugues human mind has crafted.

1
Introduction

> The central conception of all modern theory in physics is 'the Hamiltonian'. If you wish to apply modern theory to any particular problem, you must start with putting the problem 'in Hamiltonian form'.
>
> – Erwin Schrödinger, *The Hamiltonian Postage Stamp*

Hamiltonian systems are at the foundation of many current physical theories, including quantum and relativistic mechanics, electromagnetism, optics, solid and fluid mechanics. Geometry as the study of observable symmetries and dynamical invariants is *de facto* the *lingua franca* of the Hamiltonian theories. The prevailing paradigm in modeling of the complex large-scale physical systems is network modeling. In many problems arising from modern science and engineering, such as multi-body systems, electrical networks and molecular dynamics, the port-based network modeling is a natural strategy of decomposing the overall system into subsystems, which are interconnected to each other through pairs of variables called ports and whose product is the power exchanged between the subsystems.

The formalism that unifies the geometric Hamiltonian and the port-based network modeling is the *port-Hamiltonian,* the central conception of the thesis at hand.

In this thesis I propose a *geometric* framework for structure-preserving discretization of distributed-parameter port-Hamiltonian systems. Employing the formalism of discrete exterior calculus, I will introduce the notion of *simplicial Dirac structures* and show that these Dirac structures provide a natural framework for the treatment of finite-dimensional port-Hamiltonian systems on simplicial manifolds. Mirroring the framework of infinite-dimensional port-Hamiltonian systems, I will supply a number of results on structural properties of port-Hamiltonian systems on simplicial complexes of arbitrary finite

dimension. By the end, I hope, it will become clear that discrete geometry, as considered in this thesis, offers a consistent theory for discretization of distributed-parameter port-Hamiltonian systems.

Before embarking on the quest of endowing a mathematical spine to these notions, let me begin by putting them into the context.

1.1 Historical Context

The theoretical paradigm of Hamiltonian systems goes back to the spring and summer of 1834 when William Rowan Hamilton wrote two famous papers[1] "On a Geometric Method in Dynamics." Drilling through the science of mechanics with his 'long analytical borer'[2], in his essays Hamilton introduced an 'auxiliary function', which he named the 'principle function', to the modern students better known as the Hamiltonian. At the end of the second essay Hamilton had derived the canonical equations of motion by rewriting the second-order Euler-Lagrange system as a set of first-order differential equations.

Hamiltonian dynamics. Prior to the publication of his essays, geometrical ray optics and dynamics had been seen as different sciences dealing with different mathematical models, but Hamilton found a beautiful theory that would connect the two at an extremely abstract level. The largely mathematical theory had practical application, at first primarily in celestial mechanics, but soon in optics, electromagnetism, solid, fluid, quantum and statistical mechanics.

Throughout the 20th century the Euler-Lagrange and the Hamiltonian formalism have been developing hand in hand. The Hamiltonian equations of motion have been generalized to systems whose configuration space is an arbitrary n-dimensional manifold $\mathcal{Q}$ instead of $\mathbb{R}^n$, extending the symplectic vector space $\mathbb{R}^{2n}$ to the symplectic manifold $T^*\mathcal{Q}$, the cotangent bundle of $\mathcal{Q}$. Further generalization has led to definition of a general (possibly infinite-dimensional) symplectic manifold (not necessarily being a cotangent bundle), and, even more general, a Poisson structure. All these formalisms have proven to be very valuable in description and analysis of all kind of physical systems (see, e.g., [1, 9, 77]). The culmination of these developments happened in the

[1] "Hamilton's *General Method in Dynamics* is the most important of all his major mathematical discoveries; it is also the one on which he spent the least time. It grew directly out of his *Theory of Systems of Rays,* and it exhibited to an extraordinary degree his ability to create rapidly an enormous body of theory almost unparalleled in generality and abstraction," writes Hamilton's biographer Thomas L. Hankins in [45].

[2] "... [Hamilton] would drill right through the science of mechanics and out the other side with his long analytical borer," William Whewell wrote to Hamilton on March 27, 1834 [45].

late 1980s and the early 1990s when Theodore Courant and Alan Weinstein proposed a formalism of *Dirac structures* that unites symplectic and Poisson geometry [22, 23].

Port-based network modeling. For modeling of large-scale physical systems it is very effective to split a system into subsystems[3] that interact with each other via port variables called *flows* and *effort* variables, whose product defines power. This method of modeling called *port-based* modeling offers a unified way to model physical systems from different physical domains, such as mechanical, electrical, thermal, and so forth. The conceptual framework that offers a systematic way of modeling general physical systems has been successfully formalized into the modeling language of *bond graphs* formulate by Henry Paynter in 1961 (see [85] and for more references [57, 18, 39]). The setting of port-based network modeling brings many advantages to modeling and system analysis in terms of reusability of subsystem models (libraries), flexibility (coarse models of subsystems may be replaced by more refined ones, leaving the rest of the system modeling unaltered), and control (by adding new subsystems as control components in order to modify the behavior to a desired one).

Port-Hamiltonian systems. As we have seen, Hamiltonian systems have their roots in analytical mechanics, but also are a constitutive element of modern geometry and dynamical systems theory. On the other hand, the network approach stems from engineering and constitutes a cornerstone of systems theory. In the mid of 1990s van der Schaft and Maschke proposed the formalism of *port-Hamiltonian systems* as a unifying framework of the Hamiltonian and the network modeling paradigm, by associating with the interconnection structure of the network a geometric structure given by a Poisson, or more generally, a Dirac structure [95, 25, 96]. The Hamiltonian dynamics is then defined with respect to this Poisson, or Dirac, structure by specifying the Hamiltonian representing the total stored energy, the energy-dissipating elements and the ports of the system. Apart from enunciating a remarkable structural unity, Poisson and Dirac geometry offers a mathematical framework that gives important insights into dynamics and physics of port-Hamiltonian systems. Moreover, the port-Hamiltonian formalism transcends the finite-dimensional scenario and has been successfully applied to study of a number of distributed-parameter systems, systems described by a set of partial differential equations.

[3]The historically proven strategy *Divide et impera,* which has been shaping the sociopolitical landscape for millennia, is the predominate trend in modeling and analysis of large-scale systems, but now without reprobated consequences.

1.2 Distributed-Parameter Port-Hamiltonian Systems

The underlying structure of open distributed-parameter dynamical systems considered in this thesis is a *Stokes-Dirac structure* [98], a type of infinite-dimensional Dirac structure, defined in terms of differential forms on a smooth finite-dimensional orientable, usually Riemannian, manifold with a *boundary*. The Stokes-Dirac structure generalizes the framework of Poisson and symplectic structures by providing a theoretical account that permits the inclusion of varying boundary variables in the boundary problem for partial differential equations. From an interconnection and control viewpoint, such a treatment of boundary conditions is essential for the incorporation of energy exchange through the boundary, since in many applications the interconnection with the environment takes place precisely through the boundary.

In the construction of the Stokes-Dirac structure, the geometrical content of the physical variables involved is expressed by identifying them with differential forms of appropriate order. The proof that the Stokes-Dirac structure is an infinite-dimensional Dirac structure is strongly grounded on the *Stokes theorem*[4], which states that the integral of an $(n-1)$-differential form ω over the boundary of an orientable n-dimensional manifold M is equal to the integral of its exterior derivative $\mathrm{d}\omega$ over the whole of M, that is,

$$\int_M \mathrm{d}\omega = \int_{\partial\Omega} \omega.$$

In the context of the Stokes-Dirac structure, as we will see in Chapter 2, the Stokes theorem enunciates a fundamental property of port-Hamiltonian systems: the increase in the energy on the domain M is equal to the power supplied to the system through the boundary ∂M. Power is the currency of port-Hamiltonian systems[5].

1.3 Motivation and Related Approaches

For numerical integration, simulation and control synthesis, it is of paramount interest to have *finite* approximations of distributed-parameter port-Hamiltonian systems that can be interconnected to one another or via the boundary

[4] This comes as no surprise as the whole exterior geometry is firmly anchored on this coolly elegant result, which better than almost anything else reconfirms the Latin motto: *Simplex sigillum veri.*

[5] This is an instance of the more general conclusion made in [36]: "Power is the universal currency of physical systems."

coupled to other systems, be they finite- or infinite-dimensional. Most of the numerical algorithms for spatial discretization of distributed-parameter systems, primarily finite difference and finite element methods, fail to capture the intrinsic system structures and properties, such as symplecticity, conservation of momenta and energy, as well as differential gauge symmetry. Furthermore, some important results, including the Stokes theorem, fail to hold numerically and thus lead to spurious results. Given the overwhelming geometric nature of port-Hamiltonian systems, the loss of fidelity to preserve some inherently topological and geometric structures of the continuous models gives a motivation to approach computations from a geometric standpoint.

The discrete approach to geometry goes back to Whitney, who in [134] introduced an isomorphism between simplicial and de Rham cohomology. More recent antecedents can be found, for instance, in [106], and also in the computational electromagnetism literature [15, 16, 41]. For a comprehensive historical summary we refer to the thesis [49] and references therein. The literature, however, seems mostly focused on discretization of systems with infinite spatial domains, boundaryless manifolds, and systems with zero boundary conditions. The goal of the thesis is to treat port-Hamiltonian systems with *nonzero* energy flow through boundary.

A notable previous attempt to resolve the problem of structure-preserving discretization of port-Hamiltonian systems is [39], where the authors employ the mixed finite element method. Their treatment is restricted to the one-dimensional telegraph equation and the two-dimensional wave equation. Although it is hinted that the same methodology applies in higher dimensions and to the other distributed-parameter systems, the results are not clear. It is worth noting that the choice of basis functions can have dramatic consequences on the numerical performance of the mixed finite element method; as the mesh is being refined, it easily may lead to an ill-conditioned finite-dimensional linear system [8]. The other undertaking on discretization of port-Hamiltonian systems can be found in [99, 100], but the treatment is purely topological and is more akin to the graph-theoretical formulation of conservation laws. Furthermore, the authors in [99, 100] do not introduce a discrete analogue of the Stokes theorem and the entire approach is tied to the goal of preserving passivity.

The approach I propose in this thesis is that of *discrete exterior calculus* [26, 27, 49, 120], which has previously been applied to variational problems naturally arising in mechanics and electromagnetism. These problems stem from a Lagrangian, rather than Hamiltonian, modeling perspective and as such they conform to a multisymplectic structure [40, 67, 68, 126], rather than

the Stokes-Dirac structure. A crucial ingredient for numerical integration is the asynchronous variational integrator for spatio-temporally discretized problems, whereas our approach spatially discretizes the Stokes-Dirac structure and allows imposing time-continuous spatially discrete dynamics.[6]

1.4 Discrete Exterior Geometry Approach

As said, when dealing with continuous aspects of port-Hamiltonian systems, the operating language of this thesis is exterior geometry. Discrete exterior calculus is the parlance used in addressing spatially discrete port-Hamiltonian systems or the process of discretization itself.

In the discrete setting, the spatial domain in the continuous theory represented by a finite-dimensional smooth manifold is replaced by a homological *simplicial* manifold. Familiar examples of such a manifold are meshes of triangles embedded in $\mathbb{R}^3$ and tetrahedra obtained by tetrahedrization of a 3-dimensional manifold. Discrete differential forms are expressed as *cochains* on the simplicial manifold, while a discrete analogue of the exterior derivative is defined to be the *coboundary operator* from algebraic topology [73, 46].

In the fashion of discrete exterior calculus, the discrete exterior derivative $\mathbf{d}$ is constructed in such a manner that the Stokes theorem is satisfied by definition. This means, given a n-chain c and a discrete $(n-1)$-form α, the *discrete Stokes theorem* states that

$$\langle \mathbf{d}\alpha, c \rangle = \langle \alpha, \partial c \rangle \,,$$

where ∂ is the boundary operator. This result is the centerpiece of discrete exterior calculus. To rephrase Spivak [119, p. 104] in the discrete context, the discrete Stokes theorem shares three important attributes with many fully evolved mathematical constructions:

1. It is simple.
2. It is clear because the terms appearing in it have been properly defined.
3. It has significant consequences.

This bedrock of discrete geometry, in the context of port-Hamiltonian systems, as will be demonstrated in Chapter 3 and 4, expresses the fundamental

[6] This apparent discrepancy between multisymplectic and the Stokes-Dirac structure-preserving discretization could be elevated by, for instance, defining Stokes-Dirac structure on a pseudo-Riemannian manifold to insure a treatment of space and time on equal footing, whilst keeping nonzero exchange through the boundary. I will very briefly address this in the final chapter.

property of port-Hamiltonian systems defined on simplicial complexes: in the absence of internal dissipation, the rate of energy change of the system inside c is equal to the power supplied through the boundary ∂c.

1.5 Contribution and Outline of the Thesis

In Chapter 2 I begin by reviewing the basic concepts of Dirac structures and port-Hamiltonian systems, as employed in the rest of the thesis. After a brief survey of finite-dimensional structures, I recall the construction of the Stokes-Dirac structure and distributed-parameter port-Hamiltonian systems, as introduced in [98]. Section 2.3 is the only instance of this thesis where I deal with Dirac structures on Hilbert spaces. The motivation for the treatment of Dirac structures in this context is that Hilbert spaces sometimes offer a more natural formulation for the underlying partial differential equation models. Following a concise review of colligation-type Dirac structures, I introduce a Stokes-Dirac structure on the L_2 de Rham complex. Some of the preliminary results of Section 2.3 were presented in [111]. In the last section of Chapter 2 I revisit an alternative formulation of port-Hamiltonian systems as classical fields on jet bundles. Without trying to be fully rigorous, in Section 2.4 I am dealing with first-order field theories which will be revisited in Chapter 5, where I derive the port-Hamiltonian systems on the Stokes-Dirac structure through symmetry reduction of port-Hamiltonian systems presented in Section 2.4.

Readers interested primarily in structure-preserving discretization may skip Section 2.3 and 2.4 and go straight to Chapter 3.

Chapter 3 builds up discrete exterior calculus on a simplicial manifold with boundary. Firstly, I review the standard notions of chains, cochains, boundary and coboundary operators on the primal mesh. Then, I introduce the notion of the dual cell complex, which is constructed in such a way that the dual of the boundary of the simplicial manifold is the boundary of the dual cell complex. This is the crucial difference between the standard discrete exterior calculus, as presented in [26, 27, 49], and the one I am dealing with in this thesis. The introduced definition of the dual cell complex allows for the augmented notion of the dual boundary operator, which is indispensable for the construction of a discrete analogue of integration by parts formula.

In Section 3.2 I introduce the key concept of this thesis, *simplicial Dirac structures*. These finite-dimensional Dirac structures on simplicial manifolds are *terminus a quo* for the formulation of port-Hamiltonian systems on simplicial manifolds. In the rest of Chapter 3 I show how simplicial Dirac structures

relate to physical examples on a 3-, 2-, and 1-dimensional manifold: Maxwell's equations on a bounded domain, a two-dimensional wave equation, and the telegraph equations. The results presented in this chapter are published in [108, 109].

Chapter 4 deals with matrix representations of simplicial Dirac structures and resulting port-Hamiltonian systems. Primal and dual cochains are identified with vectors, while the linear operators such as discrete exterior derivative and the discrete Hodge operators are matrices. The port-Hamiltonian systems defined with respect to simplicial Dirac structures in this chapter assume the standard input-output format. When the system exhibits linear dynamics, Section 4.4 provides some guidelines how to establish bounds for the energy of discretization errors. At the end of Chapter 4 I look at a simple control strategy by energy shaping for the obtained port-Hamiltonian systems. The principle source of the material presented is [110, 113].

Chapter 5 deals with symmetry reduction of port-Hamiltonian systems. In this chapter I am looking at the Poisson reduction as proposed in [127] for closed Hamiltonian systems. In order to cope with Dirac structures on a manifold with boundary, I look at the Poisson reduction on an augmented cotangent bundle. Firstly, I obtain the Stokes-Dirac structure through symmetry reduction of a generalized canonical Dirac structure, and then apply the same methodology in the discrete world. The main source of the material presented in this chapter is [112].

In Chapter 6 I offer a geometric formulation of reaction-diffusion equations as port-Hamiltonian systems. The geometric content of the reaction-diffusion system is expressed with a Stokes-Dirac type structure on a manifold with boundary. In this way, reaction-diffusion systems are treated as a boundary controlled port-Hamiltonian system. In Section 6.5 I supply a result that certifies the spatial uniformity of the asymptotic behavior of a class of balanced reaction networks under the influence of diffusion. Then, in Section 6.6 I proceed to structure-preserving discretization of reaction-diffusion systems. Employing the methodology of Chapter 4, structured spatial discretization of reaction-diffusion systems results in a standard compartmental model. For the resulting compartmental model I provide a result that guarantees the spatiotemporal consensus of a large class of balanced reaction networks. Most of the results presented in this chapter are extensions of those in [107, 114, 115].

The last chapter, for the benefit of those who only read introductions and conclusions, summarizes what has been accomplished. I then continue to list a number of open problems, and, in my opinion, interesting research avenues.

2

Dirac Structures and Port-Hamiltonian Systems

> It seems to be one of the fundamental features of nature that fundamental physical laws are described in terms of a mathematical theory of great beauty and power, needing quite a high standard of mathematics for one to understand it. You may wonder: Why is nature constructed along these lines? One can only answer that our present knowledge seems to show that nature is so constructed. We simply have to accept it. One could perhaps describe the situation by saying that God is a mathematician of a very high order, and He used very advanced mathematics in constructing the universe. Our feeble attempts at mathematics enable us to understand a bit of the universe, and as we proceed to develop higher and higher mathematics we can hope to understand the universe better.
>
> – Paul Dirac, *The Evolution of the Physicist's Picture of Nature*

A large class of physical systems percolating down from mechanics and electromagnetism exhibit a remarkable structural unity enunciated by Dirac structures. Dirac structures were originally introduced by Courant and Weinstein in [22] as a generalization of symplectic, presymplectic and Poisson structures. The theory of Dirac structures was later developed by Courant [23] and Dorfman [29]. Soon after that the formalism of Dirac structure was employed as the geometric notion underpinning generalized power-conserving interconnections and thus allowing the Hamiltonian formulation of interconnected and constrained dynamical systems [25], [96], [98]. The open dynamical systems defined with respect to these structures belong to the class of so-called port-Hamiltonian systems. Apart from offering a geometric content of port-Hamiltonian systems, Dirac structures supply a useful framework for control synthesis of physical systems [78].

Much is known about finite-dimensional Dirac structures and their role in physics; however, hitherto there is no complete theory of Dirac structures for field theories. An initial contribution in this direction is made in by van der Schaft and Maschke in the paper [98], where the authors introduce the notion of the Stokes-Dirac structure. This infinite-dimensional Dirac structure lays down the foundation for port-Hamiltonian formulation of a class of distributed-parameter systems with boundary energy flow.

The Stokes-Dirac structure is the central gadget for the geometric treatment of the open infinite-dimensional systems in this thesis. For that reason, after brief notational preliminaries, we recall the definition of the Stokes-Dirac structure and port-Hamiltonian systems in the smooth context. This thesis for the most part treats distributed-parameter port-Hamiltonian systems on smooth manifolds; nevertheless, in this chapter we also, for the first time, introduce the notion of Stokes-Dirac structure on Hilbert spaces. Most results pertaining to port-Hamiltonian systems on the de Rham complex, namely sections 5, 6 and 7, can be shown independently; however, I have chosen to introduce them through the light of Kurula and collaborators' framework [60]. The carrier spaces of the Stokes-Dirac structures are not abstract Hilbert spaces as in [60], but are now the Hilbert spaces of differential forms on a Riemannian manifold with a Lipschitz boundary.

The last section of this chapter concerns the formulation of port-Hamiltonian systems on jet bundles. This approach, while different from the Stokes-Dirac framework, nonetheless has some common tangential points with the Dirac side. The connection of these two formulations, in a rather limited context, will be studied in Chapter 5.

2.1 Background of Port-Hamiltonian Systems

Let $\mathcal{X}$ be a manifold with tangent bundle $T\mathcal{X}$ and cotangent bundle $T^*\mathcal{X}$. We define $T\mathcal{X} \oplus T^*\mathcal{X}$ as the smooth vector bundle over $\mathcal{X}$ with fiber at each $x \in \mathcal{X}$ given by $T_x\mathcal{X} \times T_x^*\mathcal{X}$. Let X be a smooth vector field and let α be a smooth one-form on $\mathcal{X}$. Given a smooth vector bundle $\mathcal{D} \subset T\mathcal{X} \oplus T^*\mathcal{X}$, we say that the pair (X, α) belongs to $\mathcal{D}$ if $(X(x), \alpha(x)) \in \mathcal{D}$ for every $x \in \mathcal{X}$. Furthermore, we define the smooth vector subbundle $\mathcal{D}^\perp \subset T\mathcal{X} \oplus T^*\mathcal{X}$ as

$$\mathcal{D}^\perp = \left\{ (X, \alpha) \in T\mathcal{X} \oplus T^*\mathcal{X} \middle| \langle \alpha | \hat{X} \rangle + \langle \hat{\alpha} | X \rangle = 0 \text{ for all } (\hat{X}, \hat{\alpha}) \in \mathcal{D} \right\}, \quad (2.1.1)$$

with $\langle | \rangle$ denoting the duality inner product between a one-form and a vector field.

Definition 2.1.1. *A Dirac structure on a manifold $\mathcal{X}$ is a smooth vector subbundle $\mathcal{D} \subset T\mathcal{X} \oplus T^*\mathcal{X}$ such that $\mathcal{D}^\perp = \mathcal{D}$.*

Remark 2.1.1. *Usually an additional integrability condition is imposed on a Dirac structure. A Dirac structure $\mathcal{D}$ is closed or integrable if it possesses the property*

$$\langle \pounds_{X_1}\alpha_2 | X_3\rangle + \langle \pounds_{X_2}\alpha_3 | X_1\rangle + \langle \pounds_{X_3}\alpha_1 | X_2\rangle = 0 \tag{2.1.2}$$

for all $(X_1, \alpha_1), (X_2, \alpha_2), (X_3, \alpha_3) \in \mathcal{D}$.

However, for the development of this thesis the notion of integrability does not play a crucial role.

Example 2.1.1. *Let $\{,\}$ be a Poisson bracket on $\mathcal{X}$ with structural matrix $J(x)$. Then the graph of $J(x)$, that is $\mathcal{D} = \{(X, \alpha) \in T\mathcal{X} \oplus T^*\mathcal{X} | X(x) = J(x)\alpha(x)$ for $x \in \mathcal{X}\}$, is a Dirac structure on $\mathcal{X}$. The Jacobi identity for $\{,\}$ is equivalent to (2.1.2).*

Example 2.1.2. *Let ω be a two-form on $\mathcal{X}$. Then $\mathcal{D} = \{(X, \alpha) \in T\mathcal{X} \oplus T^*\mathcal{X} | i_X\omega = \alpha\}$ is a Dirac structure on $\mathcal{X}$, which satisfies (2.1.2), if and only if $\mathrm{d}\omega = 0$.*

Definition 2.1.2. *Let $\mathcal{X}$ be a manifold with Dirac structure $\mathcal{D}$ and let $H : \mathcal{X} \to \mathbb{R}$ be a smooth function, the Hamiltonian. The implicit Hamiltonian system corresponding to $(\mathcal{X}, \mathcal{D}, H)$ is given by the specification*

$$(\dot{x}, \mathrm{d}H(x)) \in \mathcal{D}, \quad x \in \mathcal{X}. \tag{2.1.3}$$

Remark 2.1.2. *Substituting $\alpha = \hat{\alpha} = \mathrm{d}H(x)$ and $X = \hat{X} = \dot{x}$ in (2.1.1) immediately leads to the energy-conservation property $\frac{\mathrm{d}H}{\mathrm{d}t} = \langle \mathrm{d}H(x) | \dot{x}\rangle = 0$.*

The notion of Dirac structures just entertained is suitable for the formulation of closed Hamiltonian systems, however, our aim is a treatment of open Hamiltonian systems in such a way that some of the external variables remain free port variables. For that reason, let $\mathcal{F}_b$ be a linear vector space of external flows, with the dual space $\mathcal{F}_b^*$ of external efforts. We deal with Dirac structures on the product space $\mathcal{X} \times \mathcal{F}_b$. The pairing on $(T\mathcal{X} \times \mathcal{F}_b) \oplus (T^*\mathcal{X} \times \mathcal{F}_b^*)$ is given by

$$\begin{aligned} &\Big\langle\Big\langle \Big((f_1, f_{b,1}), (e_1, e_{b,1})\Big), \Big((f_2, f_{b,2}), (e_2, e_{b,2})\Big)\Big\rangle\Big\rangle \\ &\quad = \langle e_1 | f_2\rangle + \langle e_{b,1} | f_{b,2}\rangle + \langle e_2 | f_1\rangle + \langle e_{b,2} | f_{b,1}\rangle \end{aligned} \tag{2.1.4}$$

for any $(f_i, f_{b,i}) \in T\mathcal{X} \times \mathcal{F}_b$ and $(e_i, e_{b,i}) \in T^*\mathcal{X} \times \mathcal{F}_b^*$, with $i = 1, 2$.

Definition 2.1.3. *A generalized Dirac structure $\mathcal{D}$ is a subbundle of $(T\mathcal{Q} \times \mathcal{F}_b) \oplus (T^*\mathcal{Q} \times \mathcal{F}_b^*)$ which is maximally isotropic under (2.1.4).*

A generalized Dirac structure (or from now on briefly, a Dirac structure) is the starting point for the geometric formulation of port-Hamiltonian systems.

Definition 2.1.4. *Consider a generalized Dirac structure $\mathcal{D}$ on the product space $\mathcal{Q} \times \mathcal{F}_b$. Let $H : \mathcal{Q} \to \mathbb{R}$ be a Hamiltonian. The **port-Hamiltonian system** corresponding to a 4-tuple $(\mathcal{Q}, \mathcal{F}_b, \mathcal{D}, H)$ is defined by*

$$(-\dot{x}(t), f(t), \mathrm{d}H(x(t)), e(t)) \in \mathcal{D} \quad \text{for } t \in I \subset \mathbb{R}. \tag{2.1.5}$$

Remark 2.1.3. *The equation (2.1.5) implies the energy balance*

$$\frac{\mathrm{d}H}{\mathrm{d}t}(x(t)) = \langle \mathrm{d}H(x(t)) | \dot{x}(t) \rangle = \langle e(t) | f(t) \rangle \quad \text{for all } t \in I.$$

The duality product of f and e represents the incoming power of the system, while the minus sign in front of $\dot{x}$ is to assure that the incoming power $\langle e, f \rangle$ is counted positively.

Example 2.1.3. *An important class of finite-dimensional port-Hamiltonian systems is given by*

$$\begin{aligned} \dot{x} &= J(x)\frac{\partial H}{\partial x}(x) + g(x)e \\ f &= g^{\mathrm{T}}(x)\frac{\partial H}{\partial x}\,, \end{aligned} \tag{2.1.6}$$

where for clarity we have omitted the argument t, and $J : T^*\mathcal{X} \to T\mathcal{X}$ is a skew-symmetric vector bundle map and $g : \mathcal{F}_b \to T\mathcal{Q}$ is the independent input vector field.

In this thesis we deal predominantly with Dirac structures on linear spaces, which can be defined as follows. Let $\mathcal{F}$ and $\mathcal{E}$ be linear spaces. Given an $f \in \mathcal{F}$ and an $e \in \mathcal{E}$, the pairing will be denoted by $\langle e | f \rangle \in \mathbb{R}$. By symmetrizing the pairing, we obtain a symmetric bilinear form $\langle\langle , \rangle\rangle : \mathcal{F} \times \mathcal{E} \to \mathbb{R}$ naturally given as $\langle\langle (f_1, e_1), (f_2, e_2) \rangle\rangle = \langle e_1 | f_2 \rangle + \langle e_2 | f_1 \rangle$.

Definition 2.1.5. *A constant Dirac structure is a linear subspace $\mathcal{D} \subset \mathcal{F} \times \mathcal{E}$ such that $\mathcal{D} = \mathcal{D}^\perp$, with $\perp$ standing for the orthogonal complement with respect to the bilinear form $\langle\langle , \rangle\rangle$.*

Remark 2.1.4. *It immediately follows that for any $(f, e) \in \mathcal{D}$*

$$0 = \langle\langle (f, e), (f, e) \rangle\rangle = 2\langle e | f \rangle\,.$$

Interpreting (f, e) as a pair of power variables, the condition $(f, e) \in \mathcal{D}$ implies power-conservation $\langle e | f \rangle = 0$.

2.2 Stokes-Dirac Structure

Throughout this section, let M be an oriented n-dimensional smooth manifold with a smooth $(n-1)$-dimensional boundary ∂M endowed with the induced orientation, representing the space of spatial variables. By $\Omega^k(M)$, $k = 0, 1, \ldots, n$, denote the space of exterior k-forms on M, and by $\Omega^k(\partial M)$, $k = 0, 1, \ldots, n-1$, the space of k-forms on ∂M. A natural non-degenerative pairing between $\alpha \in \Omega^k(M)$ and $\beta \in \Omega^{n-k}(M)$ is given by $\langle \beta | \alpha \rangle = \int_M \beta \wedge \alpha$. Likewise, the pairing on the boundary ∂M between $\alpha \in \Omega^k(\partial M)$ and $\beta \in \Omega^{n-k-1}(\partial M)$ is given by $\langle \beta | \alpha \rangle = \int_{\partial M} \beta \wedge \alpha$.

For any pair p, q of positive integers satisfying $p + q = n + 1$, define the flow and effort linear spaces by

$$\begin{aligned} \mathcal{F}_{p,q} &= \Omega^p(M) \times \Omega^q(M) \times \Omega^{n-p}(\partial M) \\ \mathcal{E}_{p,q} &= \Omega^{n-p}(M) \times \Omega^{n-q}(M) \times \Omega^{n-q}(\partial M)\,. \end{aligned}$$

The bilinear form on the product space $\mathcal{F}_{p,q} \times \mathcal{E}_{p,q}$ is given by

$$\begin{aligned} &\langle\!\langle (\underbrace{f_p^1, f_q^1, f_b^1}_{\in \mathcal{F}_{p,q}}, \underbrace{e_p^1, e_q^1, e_b^1}_{\in \mathcal{E}_{p,q}}), (f_p^2, f_q^2, f_b^2, e_p^2, e_q^2, e_b^2) \rangle\!\rangle = \\ &\int_M \left(e_p^1 \wedge f_p^2 + e_q^1 \wedge f_q^2 + e_p^2 \wedge f_p^1 + e_q^2 \wedge f_q^1 \right) + \int_{\partial M} \left(e_b^1 \wedge f_b^2 + e_b^2 \wedge f_b^1 \right)\,. \end{aligned} \tag{2.2.1}$$

Theorem 2.2.1 (Stokes-Dirac structure [98])**.** *Given linear spaces $\mathcal{F}_{p,q}$ and $\mathcal{E}_{p,q}$, and bilinear form $\langle\!\langle , \rangle\!\rangle$, define the following linear subspace $\mathcal{D}$ of $\mathcal{F}_{p,q} \times \mathcal{E}_{p,q}$*

$$\begin{aligned} \mathcal{D} = \big\{ (f_p, f_q, f_b, e_p, e_q, e_b) \in \mathcal{F}_{p,q} \times \mathcal{E}_{p,q} \big| \\ \begin{pmatrix} f_p \\ f_q \end{pmatrix} = \begin{pmatrix} 0 & (-1)^{pq+1}\mathrm{d} \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix}, \\ \begin{pmatrix} f_b \\ e_b \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -(-1)^{n-q} \end{pmatrix} \begin{pmatrix} e_p|_{\partial M} \\ e_q|_{\partial M} \end{pmatrix} \big\}\,, \end{aligned} \tag{2.2.2}$$

where d *is the exterior derivative and* $|_{\partial M}$ *stands for a trace on the boundary* ∂M*. Then* $\mathcal{D} = \mathcal{D}^\perp$*, that is,* $\mathcal{D}$ *is a Dirac structure.*

In order to define Hamiltonian dynamics, consider a Hamiltonian density $\mathcal{H} : \Omega^p(M) \times \Omega^q(M) \to \Omega^n(M)$ resulting with the Hamiltonian $H = \int_M \mathcal{H} \in \mathbb{R}$. Now, consider a time function $t \mapsto (\alpha_p(t), \alpha_q(t)) \in \Omega^p(M) \times \Omega^q(M)$, $t \in \mathbb{R}$, and the Hamiltonian $t \mapsto H(\alpha_p(t), \alpha_q(t))$ evaluated along this trajectory, then at any t

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \int_M \delta_p H \wedge \frac{\partial \alpha_p}{\partial t} + \delta_q H \wedge \frac{\partial \alpha_q}{\partial t}\,,$$

where $(\delta_p H, \delta_q H) \in \Omega^{n-p}(M) \times \Omega^{n-q}(M)$ are the (partial) variational derivatives of H at (α_p, α_q).

Setting the flows $f_p = -\frac{\partial \alpha_p}{\partial t}$, $f_q = -\frac{\partial \alpha_q}{\partial t}$ and the efforts $e_p = \delta_p H$, $e_q = \delta_q H$, the ***distributed-parameter port-Hamiltonian system*** is defined by the relation

$$\left(-\frac{\partial \alpha_p}{\partial t}, -\frac{\partial \alpha_q}{\partial t}, f_b, \delta_p H, \delta_q H, e_b\right) \in \mathcal{D}. \tag{2.2.3}$$

Remark 2.2.1. *For the port-Hamiltonian system (2.2.3), it straightaway follows that* $\frac{dH}{dt} = \int_{\partial M} e_b \wedge f_b$*, expressing the fact that the system is lossless. In other words, the increase in the energy of the system is equal to the power supplied to the system through the boundary* ∂M*.*

The spaces of differential forms $\Omega^p(M)$ and $\Omega^q(M)$, as we see from the formulation of port-Hamiltonian system, represent the energy variables of two different physical energy domains interacting with each other, while $\Omega^{n-p}(\partial M)$ and $\Omega^{n-q}(\partial M)$ stand for the boundary variables whose product represents the boundary energy flow. For example, in Maxwell's equation we have $n = 3$ and $p = q = 2$; that is, $\Omega^p(M) = \Omega^2(M)$ and $\Omega^q(M) = \Omega^2(M)$ being the space of electric field inductions and the space of magnetic field inductions, respectively, while $\Omega^{n-p}(\partial M) = \Omega^2(\partial M)$ denote the electric and magnetic field intensities at the boundary with product being the Poynting vector [98].

2.3 Dirac Structures on Hilbert Spaces

In the previous section we have covered the basic ingredients for the formulation of port-Hamiltonian systems on smooth configuration spaces. Sometimes the smooth formulation is too restrictive. For instance, the boundary interconnection of two smooth port-Hamiltonian systems, in general, is not a port-Hamiltonian system on a smooth manifold. Hilbert spaces offer a framework general enough to cover problems similar to this one and at the same time supply ample tools for their analysis.

Dirac structures in the context of Hilbert spaces previously were studied in [39, 37, 60, 53]. The underlying spaces were Hilbert spaces of functions. Our goal in this section is to identify the geometric content of the underlying Hilbert spaces. For that purpose, we firstly recall the essentials of the Hilbert spaces of differential forms, and then we review the necessary notation and results from [60]. Here we deal with the so-called colligation-type Dirac structures on abstract Hilbert spaces. This formulation turns out to be sufficiently general to cover the Stokes-Dirac structure, so the only novelty is that I identify the appropriate Hilbert spaces. The L^2 spaces of differential forms are the

carrier spaces of the Stokes-Dirac structure on the de Rham complex. At the end of the section I show that the boundary composition of two Stokes-Dirac structures is again a Dirac structure.

2.3.1 The de Rham Complex as a Hilbert Complex

We review the basic notions of a Hilbert complex on a Riemannian manifold with boundary. Much more can be found in [7, 8, 9, 17, 31, 55, 61, 122]. The first subsection 2.3.1 is strongly based on Section 2 of [8].

Henceforth, we restrict attention to the case when M is a bounded domain in $\mathbb{R}^n$ with a piecewise smooth, Lipschitz boundary. In this section we show that the de Rham complex is a Hilbert complex which satisfies the compactness property.

On an oriented Riemannian manifold, the Sobolev spaces $H^s(M)$ and $W_p^s(M)$ are the spaces of functions with $s \geq 0$ derivatives in $L^2(M)$ and $L^p(M)$. In the literature, the spaces $H^s\Omega^k(M)$ are Hilbert spaces of differential forms for which all their partial derivatives of order at most s, in some coordinate system, are square integrable.

Analogously, $H\Omega^k(M)$ is defined to be the space of forms in $L^2\Omega^k(M)$ with a weak exterior derivative in $L^2\Omega^{k+1}(M)$, that is

$$H\Omega^k(M) = \left\{\omega \in L^2\Omega^k(M) \,|\, \mathrm{d}\omega \in L^2\Omega^{k+1}(M)\right\}$$

with the norm defined as

$$\|\omega\|^2_{H\Omega^k(M)} = \|\omega\|^2_{L^2\Omega^k(M)} + \|\mathrm{d}\omega\|^2_{L^2\Omega^{k+1}(M)}\,.$$

The space $H\Omega^0(M)$ is in fact $H^1\Omega^0(M)$, or simply $H^1(M)$, while $H\Omega^n(M)$ coincides with $L^2\Omega^n(M)$. For $0 < k < n$, $H^1\Omega^k(M) \subseteq H\Omega^k(M) \subseteq L^2\Omega^k(M)$.

Standard smoothing arguments imply that $C^\infty\Omega^k(M)$ is dense in $H\Omega^k(M)$. Taking $H\Omega^k(M)$ for the domain of the exterior derivative, this operator is densely defined in $L^2\Omega^k(M)$. Since $H\Omega^k$ is complete, d is a closed operator. The spaces $L^2\Omega^k(M)$, together with the exterior derivative d, form a Hilbert complex

$$0 \to H\Omega^0(M) \xrightarrow{\mathrm{d}} H\Omega^1(M) \xrightarrow{\mathrm{d}} \cdots \xrightarrow{\mathrm{d}} H\Omega^n(M) \to 0. \tag{2.3.1}$$

This is the L^2 de Rham complex.

Similarly to definition of $H\Omega^k(M)$, we define

$$H^*\Omega^k(M) = \left\{\omega \in L^2\Omega^k(M) \,|\, \delta\omega \in L^2\Omega^{k-1}(M)\right\},$$

where δ is the coderivative operator $\delta : \Omega^k(M) \to \Omega^{k-1}(M)$ defined by

$$* \, \delta\omega = (-1)^k \mathrm{d} * \omega, \tag{2.3.2}$$

with $*$ being the Hodge star operator and $\omega \in \Omega^k(M)$.

Since $H^*\Omega^k(M)$ is isometric to $H\Omega^{n-k}$, the dual de Rham complex is

$$0 \leftarrow H^*\Omega^0(M) \xleftarrow{\delta} H^*\Omega^1(M) \xleftarrow{\delta} \cdots \xleftarrow{\delta} H^*\Omega^n(M) \leftarrow 0.$$

Trace operators. The trace operator $\mathrm{tr} : \Omega^k(M) \to \Omega^k(\partial M)$ extends by continuity to a mapping of $H^1\Omega^k(M)$ onto the Sobolev space $H^{1/2}\Omega^k(\partial M)$. The trace cannot be extended to all $L^2\Omega^k(M)$, but it is possible to give a meaning to the trace of $\omega \in H\Omega^k(M)$. Following Arnold, Falk and Winther [8], let $\rho \in H^{1/2}\Omega^k(\partial M)$, and let $\bar{*}\rho \in H^{1/2}\Omega^{n-k-1}(\partial M)$ be the Hodge star of ρ with respect to the boundary. Then, there is $\eta \in H^1\Omega^{n-k-1}(M)$ with $\mathrm{tr}\,\eta = \bar{*}\rho$, and

$$\|\eta\|_{H^1\Omega^{k-1}(M)} \leq c\|\bar{*}\rho\|_{H^{1/2}\Omega^{n-k-1}(\partial M)} \leq c\|\rho\|_{H^{1/2}\Omega^{n-k-1}(\partial M)}\,.$$

For $\omega \in \Omega^k(M)$, employing the integration by parts formula, we have

$$\begin{aligned}\langle \mathrm{tr}\,\omega, \rho\rangle &= \int_{\partial M} \mathrm{tr}\,\omega \wedge \bar{*}\rho = \int_{\partial M} \mathrm{tr}\,\omega \wedge \mathrm{tr}\,\eta \\ &= \int_M \Big(\mathrm{d}\omega \wedge \eta + (-1)^k \wedge \mathrm{d}\eta\Big) \leq c\|\omega\|_{H\Omega}\|\eta\|_{H^1} \\ &\leq c\|\omega\|_{H\Omega}\|\rho\|_{H^{1/2}}\,.\end{aligned}$$

This implies that the trace operator extends boundedly from $H\Omega^k(M)$ to $H^{-1/2}\Omega^k(\partial M)$, the dual of $H^{1/2}\Omega^k(\partial M)$.

The integration by parts formula in the context of Hilbert spaces is

$$\langle \mathrm{d}\omega, \mu\rangle = \langle \omega, \delta\mu\rangle + \int_{\partial M} \mathrm{tr}\,\omega \wedge \mathrm{tr} * \mu, \quad \omega \in H\Omega^{k-1}(M),\ \mu \in H^1\Omega^k(M). \tag{2.3.3}$$

Because of the isometry between $H^*\Omega^k(M)$ and $*(H\Omega^{n-k})$, (2.3.3) holds also for $\omega \in H^1\Omega^{k-1}(M)$ and $\mu \in H^*\Omega^k(M)$.

Here it is important to emphasize that for a smooth k-form ω, $\mathrm{tr}\,\omega$ vanishes if and only if its tangential part vanishes, while $\mathrm{tr}\,(*\omega)$ vanishes if and only if its normal part vanishes.

Vetor calculus aspects. On any oriented Riemannian manifold of dimension n, we have a natural way to view 0-forms and n-forms as real-valued functions,

and 1-forms and $(n-1)$-forms as vector fields. In fact, 0-forms are real-valued functions and 1-forms are covector fields, which can be identified with vector fields via the inner product. The Hodge star operation then carries these identifications to n-forms and $(n-1)$-forms. In the case of a 3-dimensional domain in $\mathbb{R}^3$, via these identifications all k-forms can be viewed as either scalar or vector fields (sometimes called *proxy fields*). With these identifications, the Hodge star operation becomes trivial in the sense if a certain vector field is the proxy for, e.g., a 1-form ω, the exact same vector field is the proxy for the 2-form $*\omega$. Via proxy fields, the exterior derivatives coincide with standard differential operators grad, curl and div, and the de Rham complex (2.3.1) is realized as

$$0 \to H^1(M) \xrightarrow{\text{grad}} H(\text{curl}; M) \xrightarrow{\text{curl}} H(\text{div}; M) \xrightarrow{\text{div}} L^2(M) \to 0,$$

where

$$H(\text{curl}; \Omega) = \{\, u : M \to \mathbb{R}^3 \,|\, u \in L^2(M),\ \ \text{curl}\, u \in L^2(M) \,\},$$
$$H(\text{div}; \Omega) = \{\, u : M \to \mathbb{R}^3 \,|\, u \in L^2(M),\ \ \text{div}\, u \in L^2(M) \,\}.$$

The exterior coderivatives δ become, of course, $-\,\text{div}$, curl, and $-\text{grad}$, when acting on 1-forms, 2-forms, and 3-forms, respectively. The trace operation on 0-forms is just the restriction to the boundary, and the trace operator on 3-forms vanishes (since there are no nonzero 3-forms on $\partial\Omega$). The trace operator from 1-forms on Ω to 1-forms on the boundary takes a vector field u on Ω to a tangential vector field on the boundary, namely at each boundary point x, $(\text{tr}\, u)_x$ is the tangential projection of u_x. For a 2-form u, the trace corresponds to the scalar $u \cdot n$ (with n the unit normal) at each boundary point.

2.3.2 Constant Dirac Structures on Hilbert Spaces

Let $\mathcal{E}$ and $\mathcal{F}$ be two Hilbert spaces to which we shall refer to as the effort space and the flow space, respectively. Assume that there is a unitary operator $\mathsf{r}_{\mathcal{E},\mathcal{F}}$ from $\mathcal{E}$ to $\mathcal{F}$ with the adjoint $\mathsf{r}^*_{\mathcal{E},\mathcal{F}}$.

By the Hilbert space $\mathcal{F} \oplus \mathcal{E}$ we consider the product space $\mathcal{F} \times \mathcal{E}$ equipped with the inner product

$$\left\langle \begin{pmatrix} f_1 \\ e_1 \end{pmatrix}, \begin{pmatrix} f_2 \\ e_2 \end{pmatrix} \right\rangle_{\mathcal{F}\oplus\mathcal{E}} = \langle f_1, f_2 \rangle_{\mathcal{F}} + \langle e_1, e_2 \rangle_{\mathcal{E}}\,, \tag{2.3.4}$$

for any $f_1, f_2 \in \mathcal{F}$ and $e_1, e_2 \in \mathcal{E}$.

The bond space $\mathcal{B}$ is defined to be a Hilbert space $\mathcal{F} \times \mathcal{E}$ equipped with the inner product $\langle , \rangle_{\mathcal{B}}$ given by

$$\left\langle \begin{pmatrix} f_1 \\ e_1 \end{pmatrix}, \begin{pmatrix} f_2 \\ e_2 \end{pmatrix} \right\rangle_{\mathcal{B}} = \left\langle \begin{pmatrix} f_1 \\ e_1 \end{pmatrix}, \begin{pmatrix} 0 & \mathsf{r}_{\mathcal{E},\mathcal{F}} \\ \mathsf{r}^*_{\mathcal{E},\mathcal{F}} & 0 \end{pmatrix} \begin{pmatrix} f_2 \\ e_2 \end{pmatrix} \right\rangle_{\mathcal{F}\oplus\mathcal{E}} \tag{2.3.5}$$
$$= \langle f_1, \mathsf{r}_{\mathcal{E},\mathcal{F}} e_2 \rangle_{\mathcal{F}} + \langle e_1, \mathsf{r}^*_{\mathcal{E},\mathcal{F}} f_2 \rangle_{\mathcal{E}} \, .$$

Given a linear subspace $\mathcal{C} \subset \mathcal{B}$, the orthogonal companion $\mathcal{C}^{\perp\!\!\!\perp}$ of $\mathcal{C}$ is defined by

$$\mathcal{C}^{\perp\!\!\!\perp} = \left\{ \bar{b} \in \mathcal{B} : \langle b, \bar{b} \rangle_{\mathcal{B}} = 0 \text{ for all } b \in \mathcal{C} \right\} . \tag{2.3.6}$$

Due to the indefinite inner product $\langle , \rangle_{\mathcal{B}}$, for any linear subspace $\mathcal{C}$ of $\mathcal{B}$ the following holds

$$\mathcal{C}^{\perp\!\!\!\perp} = \begin{pmatrix} 0 & \mathsf{r}_{\mathcal{E},\mathcal{F}} \\ \mathsf{r}^*_{\mathcal{E},\mathcal{F}} & 0 \end{pmatrix} \mathcal{C}^{\perp} \, , \tag{2.3.7}$$

where $\mathcal{C}^{\perp}$ stands for the orthogonal complement of $\mathcal{C}$ with respect to the scalar product $\langle , \rangle_{\mathcal{F}\oplus\mathcal{E}}$. Since the inner product $\langle , \rangle_{\mathcal{B}}$ is non-degenerate, any orthogonal companion of $\mathcal{C}$ is closed.

Definition 2.3.1. *A Dirac structure $\mathcal{D}$ of the bond space $\mathcal{B}$ is a subspace $\mathcal{D} \subset \mathcal{B}$ which is maximally isotropic under the inner product $\langle , \rangle_{\mathcal{B}}$, that is $\mathcal{D} = \mathcal{D}^{\perp\!\!\!\perp}$.*

Colligation-type Dirac structures on Hilbert spaces. In this section we lay down the framework for the analysis of Dirac structures in the context of Hilbert spaces.

Definition 2.3.2 ([60])**.** *Given three Hilbert spaces U, X, Y, let G, L, K be linear operators, with common domain in X, that map into U, X, and Y, respectively.*

1. *The pair $\left(\begin{pmatrix} G \\ L \\ K \end{pmatrix}, \begin{pmatrix} U \\ X \\ Y \end{pmatrix} \right)$ is called an operator colligation or colligation.*

2. *The colligation is said to be strong if $\Xi = \begin{pmatrix} G \\ L \\ K \end{pmatrix}$ and L are closed operators, with domain $\mathrm{dom}(L) = \mathrm{dom}(\Xi)$.*

3. The minimal (interior) operator of Ξ *is defined as*

$$L_0 = L|_{\{x\in \mathrm{dom} L | Kx=0, Gx=0\}}\,.$$

When the spaces are clear from the context, the operator Ξ *will be called colligation.*

Assume that the Hilbert spaces U and Y have the same cardinality. This allows as to fix a unitary map $\mathsf{r}_{U,Y}$ between U and Y. Introduce the effort and flow spaces as

$$\mathcal{E} = X \oplus U \quad \text{and} \quad \mathcal{F} = X \oplus Y\,. \tag{2.3.8}$$

The unitary mapping from $\mathcal{E}$ to $\mathcal{F}$ is

$$\mathsf{r}_{\mathcal{E},\mathcal{F}} = \begin{pmatrix} \mathsf{id} & 0 \\ 0 & -\mathsf{r}_{U,Y} \end{pmatrix}, \tag{2.3.9}$$

where id is the identity operator in X.

The indefinite power product on the bond space $\mathcal{B} = \mathcal{F} \times \mathcal{E}$ is given by

$$\begin{aligned}\left\langle \begin{pmatrix} z_1 \\ y_1 \\ x_1 \\ u_1 \end{pmatrix}, \begin{pmatrix} z_2 \\ y_2 \\ x_2 \\ u_2 \end{pmatrix} \right\rangle_{\mathcal{B}} =& \langle z_1, x_2\rangle_X - \langle y_1, \mathsf{r}_{U,Y} u_2\rangle_Y \\ &+ \langle x_1, z_2\rangle_X - \langle u_1, \mathsf{r}^*_{U,Y} y_2\rangle_U\,,\end{aligned} \tag{2.3.10}$$

where $x_1, z_1, x_2, z_2 \in X$, $y_1, y_2 \in Y$, and $u_1, u_2 \in U$. Let $\left(\begin{pmatrix} G \\ L \\ K \end{pmatrix}, \begin{pmatrix} U \\ X \\ Y \end{pmatrix}\right)$ be a colligation defined on $\mathrm{dom}(\Xi)$ as specified in Definition 2.3.2. Consider the space $\mathcal{D}$ defined by

$$\mathcal{D} = \begin{pmatrix} L \\ K \\ \mathsf{id} \\ G \end{pmatrix} \mathrm{dom}(\Xi) \subset \mathcal{F} \times \mathcal{E} = (X \oplus Y) \times (X \oplus U)\,. \tag{2.3.11}$$

The following proposition from [60] gives the conditions for $\mathcal{D}$ to be contained in $\mathcal{D}^{\perp\!\!\!\perp}$.

Proposition 2.3.1 ([60]). *Let the bond space $\mathcal{B} = \mathcal{F} \times \mathcal{E}$ with the power product as in (2.3.8)–(2.3.10), and let $\mathcal{D}$ be defined by (2.3.11). Then, $\mathcal{D} \subset \mathcal{D}^{\perp\!\!\!\perp}$ if and only if*

$$\langle Lx, x\rangle_X = \langle Kx, r_{U,Y} Gx\rangle_Y, \quad x \in \operatorname{dom}(\Xi). \tag{2.3.12}$$

The main result from [60] supplies necessary and sufficient conditions for $\mathcal{D}$ to be a Dirac structure.

Theorem 2.3.2 ([60]). *Given the bond space $\mathcal{B} = \mathcal{F} \times \mathcal{E}$ with the power product be as in (2.3.8)–(2.3.10), let $\mathcal{D}$ be defined as in (2.3.11), and assume that the operator L is closed. The space $\mathcal{D}$ is a Dirac structure on $\mathcal{B}$ if and only if the following holds:*

1. *Equation (2.3.12) is satisfied.*
2. *The minimal operator L_0 is densely defined and $L_0^* = -L$ holds.*
3. *The range of the operator $\begin{pmatrix} G \\ K \end{pmatrix}$ is dense in $U \oplus Y$.*

Composition of Dirac structures. Consider two Dirac structures $\mathcal{D}_A$ and $\mathcal{D}_B$ respectively defined on two n-dimensional manifolds M_A and M_B, such that

$$\begin{aligned} \partial M_A &= \Gamma \cup \Gamma_A\,, \quad \Gamma \cap \Gamma_A = \emptyset\,, \\ \partial M_B &= \Gamma \cup \Gamma_B\,, \quad \Gamma \cap \Gamma_B = \emptyset\,, \end{aligned}$$

for certain $(n-1)$-dimensional manifolds $\Gamma, \Gamma_A, \Gamma_B$ (see Figure 1). This means that the boundaries ∂M_A and ∂M_B share a common $(n-1)$-dimensional manifold Γ. The two structures $\mathcal{D}_A$ and $\mathcal{D}_B$ compose a Dirac structure on $M_A \cup M_B \cup \Gamma$ with boundary $\Gamma_A \cup \Gamma_B$.

Let $j \in \{A, B\}$, let U^j, X^j, and Y^j be Hilbert spaces and assume that U^j and Y^j are split into $U^j = U_b^j \oplus U_c$ and $Y^j = Y_b^j \oplus Y_c$. Let G^j, L^j, and K^j be linear operators with common domain $\operatorname{dom} \Xi^j$ dense in X^j that map into U^j, X^j, and Y^j, respectively. Split G^j and K^j according to the decomposition of U^j and Y^j into

$$G^j = \begin{pmatrix} G_b^j \\ G_c^j \end{pmatrix} \quad \text{and} \quad K^j = \begin{pmatrix} K_b^j \\ K_c^j \end{pmatrix}. \tag{2.3.13}$$

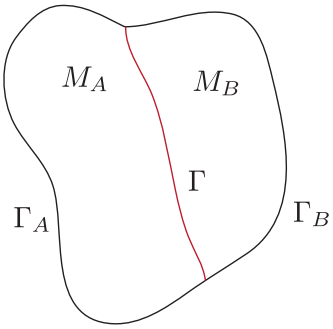


Figure 2.1: Composition of two Stokes-Dirac structures through the associated boundary.

There exist the unitary operators

$$\mathsf{r}_{U^j,Y^j} = \begin{pmatrix} \mathsf{r}_{U_b^j,Y_b^j} & 0 \\ 0 & \mathsf{r}_{U_c,Y_c} \end{pmatrix} : \begin{pmatrix} U_b^j \\ U_c \end{pmatrix} \to \begin{pmatrix} Y_b^j \\ Y_c \end{pmatrix} . \tag{2.3.14}$$

The colligations

$$\Xi^j = \begin{pmatrix} G_b^j \\ G_c^j \\ L^j \\ K_b^j \\ K_c^j \end{pmatrix} \quad \text{for } j = A, B, \tag{2.3.15}$$

are defined on the dense subspaces $\operatorname{dom}\Xi^j$ of X^j.

This leads to the following set-up for split Dirac structures:

$$\mathcal{E}^j = \begin{pmatrix} X^j \\ U_b^j \end{pmatrix} , \ \mathcal{F}^j = \begin{pmatrix} X^j \\ Y_b^j \end{pmatrix} , \ \mathcal{E}_2 = U_c \ \ \mathcal{F}_2 = Y_c , \ j = A, B. \tag{2.3.16}$$

Set $\mathcal{B}^j = \mathcal{F}^j \oplus \mathcal{F}^2 \times \mathcal{E}^j \oplus \mathcal{E}_2$, and define the subspace $\mathcal{D}^j \subset \mathcal{B}^j$ as

$$\mathcal{D}^j = \begin{pmatrix} L^j \\ K_b^j \\ K_c^j \\ \mathsf{id} \\ G_b^j \\ G_c^j \end{pmatrix} \operatorname{dom}\Xi^j , \quad j = A, B. \tag{2.3.17}$$

The composition of $\mathcal{D}^A$ and $\mathcal{D}^B$ is done by setting $f_2^A = -f_2^B$ and $e_2^A = e_2^B$, that is

$$K_c^A x^A + K_c^B x^B = 0 \quad \text{and} \quad G_c^A x^A = G_c^B x^B \tag{2.3.18}$$

for $x^A \in \operatorname{dom} \Xi^A$ and $x^B \in \operatorname{dom} \Xi^B$. Introduce the subspace

$$\operatorname{dom} \Xi^{AB} = \left\{ \begin{pmatrix} x^A \\ x^B \end{pmatrix} \,\middle|\, x^j \in \operatorname{dom} \Xi^j \text{ and (2.3.18) holds} \right\} \tag{2.3.19}$$

of $X^A \oplus X^B$, the operators

$$\begin{aligned} G^{AB} &= \begin{pmatrix} G_b^A & 0 \\ 0 & G_b^B \end{pmatrix} : \operatorname{dom} \Xi^{AB} \to U_b^A \oplus U_b^B, \\ L^{AB} &= \begin{pmatrix} L^A & 0 \\ 0 & G^B \end{pmatrix} : \operatorname{dom} \Xi^{AB} \to X^A \oplus X^B, \\ K^{AB} &= \begin{pmatrix} K_b^A & 0 \\ 0 & K_b^B \end{pmatrix} : \operatorname{dom} \Xi^{AB} \to Y_b^A \oplus Y_b^B, \end{aligned} \tag{2.3.20}$$

and the colligation $\Xi^{AB} = \begin{pmatrix} G^{AB} \\ L^{AB} \\ K^{AB} \end{pmatrix}$.

Theorem 2.3.3 ([60]). *Assume that the colligations Ξ^A and Ξ^B defined by (2.3.15) are strong and that $\mathcal{D}^A$ and $\mathcal{D}^B$ in (2.3.15) are Dirac structures. Then*

$$\mathcal{D}^A \circ \mathcal{D}^B = \begin{pmatrix} L^{AB} \\ K^{AB} \\ \mathsf{id} \\ G^{AB} \end{pmatrix} \operatorname{dom} \Xi^{AB} \tag{2.3.21}$$

is a Dirac structure associated with the strong colligation Ξ^{AB} with the unitary map

$$r_{\mathcal{E},\mathcal{F}} = \begin{pmatrix} \mathsf{id}_{X^A} & 0 & 0 & 0 \\ 0 & \mathsf{id}_{X^B} & 0 & 0 \\ 0 & 0 & -r_{U_b^A, Y_b^A} & 0 \\ 0 & 0 & 0 & -r_{U_b^B, Y_b^B} \end{pmatrix}. \tag{2.3.22}$$

In the next section we shall apply the results presented here in the context of the Stokes-Dirac structure on the L^2 de Rham complex.

2.3.3 The Stokes-Dirac Structure on the de Rham Complex

Let the configuration space be $X_{p,q} = L^2\Omega^{k-1}(M) \oplus L^2\Omega^k(M)$. Introduce the space of boundary efforts $\mathcal{E}_b = H^{-1/2}\Omega^{k-1}(\partial M)$ and let the space of boundary flows be $\mathcal{F}_b = H^{1/2}\Omega^{n-k}(\partial M)$. The complete spaces of efforts and flows are given as

$$\mathcal{E}_{p,q} = X_{p,q} \oplus \mathcal{E}_b \quad \text{and} \quad \mathcal{F}_{p,q} = X_{p,q} \oplus \mathcal{F}_b\,. \tag{2.3.23}$$

The unitary mapping from $\mathcal{E}_{p,q}$ to $\mathcal{F}_{p,q}$ is

$$\mathsf{r}_{\mathcal{E}_{p,q},\mathcal{F}_{p,q}} = \begin{pmatrix} \mathsf{id} & 0 \\ 0 & -\bar{*} \end{pmatrix}, \tag{2.3.24}$$

where id is the identity operator in $L^2\Omega^{k-1}(M) \oplus L^2\Omega^k(M)$ and $\bar{*}$ is the Hodge operator on the boundary ∂M.

The bilinear form on the bond space $\mathcal{B}_{p,q} = \mathcal{F}_{p,q} \times \mathcal{E}_{p,q}$ is

$$\begin{aligned} \left\langle \begin{pmatrix} f_p^1 \\ f_q^1 \\ f_b^1 \\ e_p^1 \\ e_q^1 \\ e_b^1 \end{pmatrix}, \begin{pmatrix} f_p^2 \\ f_q^2 \\ f_b^2 \\ e_p^2 \\ e_q^2 \\ e_b^2 \end{pmatrix} \right\rangle_{\mathcal{B}_{p,q}} &= \langle f_p^1, e_p^2 \rangle_{L^2\Omega^{k-1}} + \langle f_q^1, e_q^2 \rangle_{L^2\Omega^k} - \langle f_b^1, *e_b^2 \rangle_{\mathcal{F}_b} \\ &\quad + \langle e_p^1, f_p^2 \rangle_{L^2\Omega^{k-1}} + \langle e_q^1, f_q^2 \rangle_{L^2\Omega^k} - \langle e_b^1, \bar{*} f_b^2 \rangle_{\mathcal{E}_b}\,, \end{aligned} \tag{2.3.25}$$

where $f_p^1, f_p^2, e_p^1, e_p^2 \in L^2\Omega^{k-1}(M)$, $f_q^1, f_q^2, e_q^1, e_q^2 \in L^2\Omega^k(M)$, and the boundary variables $f_b^1, f_b^2 \in H^{1/2}\Omega^{n-k}(\partial M)$ and $e_b^1, e_b^2 \in H^{-1/2}\Omega^{k-1}(\partial M)$.

By now we have all the necessary ingredients for the (re)formulation of the Stokes-Dirac structure on the de Rham complex.

Theorem 2.3.4. *Given linear spaces $\mathcal{F}_{p,q}$ and $\mathcal{E}_{p,q}$, and bilinear form $\langle , \rangle_{\mathcal{B}_{p,q}}$, define the following linear subspace $\mathcal{D}_{p,q}$ of $\mathcal{F}_{p,q} \times \mathcal{E}_{p,q}$*

$$\begin{aligned} \mathcal{D}_{p,q} = \big\{ (f_p, f_q, f_b, e_p, e_q, e_b) \in \mathcal{F}_{p,q} \times \mathcal{E}_{p,q} \big| \\ \begin{pmatrix} f_p \\ f_q \end{pmatrix} = \begin{pmatrix} 0 & -\delta \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix}, \\ \begin{pmatrix} e_b \\ f_b \end{pmatrix} = \begin{pmatrix} \mathrm{tr} & 0 \\ 0 & \mathrm{tr}\,* \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix}, \\ \text{such that } (e_p, e_q) \in H\Omega^{k-1}(M) \oplus H^1\Omega^k(M) \big\}\,. \end{aligned} \tag{2.3.26}$$

Then $\mathcal{D}_{p,q} = \mathcal{D}_{p,q}^{\perp\!\!\!\perp}$, that is, $\mathcal{D}_{p,q}$ is a Dirac structure.

Proof. For the proof we shall use the 'if' part of Theorem 2.3.2. To this end, we identify the following operators: $L = \begin{pmatrix} 0 & -\delta \\ \mathrm{d} & 0 \end{pmatrix}$, $G = \begin{pmatrix} \mathrm{tr} & 0 \end{pmatrix}$ and $K = \begin{pmatrix} 0 & \mathrm{tr}\,* \end{pmatrix}$.

Observe that $\operatorname{dom} L = H\Omega^{k-1}(M) \oplus H^1\Omega^k(M) = \operatorname{dom} \Xi$. The operators L and $\Xi = \begin{pmatrix} G \\ L \\ K \end{pmatrix}$ are closed in L^2 (since all the operators in L, G and K are, see [7, 8]), thus Ξ is a strong colligation (cf. Definition 2.3.2).

The minimal operator of Ξ is

$$L_0 = L|_{\left\{(e_p,e_q)\in H\Omega^{k-1}(M)\oplus H^1\Omega^k(M) \,|\, \mathrm{tr}\, e_p = 0, \mathrm{tr}\, *e_q = 0\right\}}. \tag{2.3.27}$$

The relation (2.3.12) in our case is

$$\left\langle L \begin{pmatrix} e_p \\ e_q \end{pmatrix}, \begin{pmatrix} e_p \\ e_q \end{pmatrix} \right\rangle_{X_{p,q}} = \left\langle \begin{pmatrix} 0 & \mathrm{tr}\,* \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix}, \bar{*} \begin{pmatrix} \mathrm{tr} & 0 \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix} \right\rangle_{\mathcal{F}_b}. \tag{2.3.28}$$

After writing out all the components, the last equation is nothing other than the integration by parts formula (2.3.3), which in the present scenario is written as

$$\begin{aligned} \langle \mathrm{d}e_p, e_q \rangle_{L^2\Omega^k} &= \langle e_p, \delta e_q \rangle_{L^2\Omega^{k-1}} + \int_{\partial M} \mathrm{tr}\, e_p \wedge \mathrm{tr}\, *\, e_q \\ &= \langle e_p, \delta e_q \rangle_{L^2\Omega^{k-1}} + \langle \mathrm{tr} * e_q, \bar{*}\mathrm{tr}\, e_p \rangle_{H^{1/2}\Omega^{n-k}}. \end{aligned} \tag{2.3.29}$$

This implies that the first condition of Theorem 2.3.2 is satisfied.

The exterior derivative d and the codifferential operator δ are dense in L^2 [8], hence the minimal operator L_0 is dense and $L_0^* = \begin{pmatrix} 0 & \delta \\ -\mathrm{d} & 0 \end{pmatrix} = -L$.

Furthermore, the trace operators $\mathrm{tr} : H\Omega^{k-1}(M) \to H^{-1/2}\Omega^{k-1}(\partial M)$ and $\mathrm{tr}* : H^1\Omega^k(M) \to H^{1/2}\Omega^{n-k}(\partial M)$ are dense in $\mathcal{E}_b$ and $\mathcal{F}_b$, respectively, and thus the third condition of Theorem 2.3.2 is fulfilled. This concludes the proof. □

2.3.4 Port-Hamiltonian Systems on the de Rham Complex

Port-Hamiltonian dynamics can be introduced in the same manner as it has been done in the smooth scenario. To that end, consider a Hamiltonian density $\mathsf{h} : L^2\Omega^{k-1}(M) \times L^2\Omega^k(M) \to L^2\Omega^n(M)$ resulting in the Hamiltonian $H = \int_M \mathsf{h} \in \mathbb{R}$. Now, consider a trajectory $t \mapsto (\alpha_p(t), \alpha_q(t)) \in L^2\Omega^{k-1}(M) \times$

$L^2\Omega^k(M)$, $t \in \mathbb{R}$, and the Hamiltonian $t \mapsto H(\alpha_p(t), \alpha_q(t))$ evaluated along this trajectory, then at any instance t

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \left\langle \delta_p H, \frac{\partial \alpha_p}{\partial t} \right\rangle_{L^2\Omega^{k-1}} + \left\langle \delta_q H, \frac{\partial \alpha_q}{\partial t} \right\rangle_{L^2\Omega^{k-1}}, \tag{2.3.30}$$

where $(\delta_p H, \delta_q H) \in H\Omega^{k-1}(M) \times H^1\Omega^k(M)$ are the variational derivatives of H at (α_p, α_q).

Specifying the flows $f_p = -\frac{\partial \alpha_p}{\partial t}$, $f_q = -\frac{\partial \alpha_q}{\partial t}$ and the efforts $e_p = \delta_p H$, $e_q = \delta_q H$ results in the distributed-parameter port-Hamiltonian system

$$\left(-\frac{\partial \alpha_p}{\partial t}, -\frac{\partial \alpha_q}{\partial t}, f_b, \delta_p H, \delta_q H, e_b \right) \in \mathcal{D}_{p,q}. \tag{2.3.31}$$

Proposition 2.3.5. *The port-Hamiltonian system (2.3.31) is lossless, that is* $\frac{dH}{dt} = \int_{\partial M} e_b \wedge f_b$. *In other words, the increase in the energy of the system (2.3.31) is equal to the power supplied to the system through the boundary* ∂M.

Now we give a physical example of the port-Hamiltonian system (2.3.31) on a two-dimensional bounded domain.

Example: Two-dimensional vibrating string. Consider the wave equation $\mu\, \partial^2/\partial t^2 u = -E\Delta u$, with $u(t, z) \in \mathbb{R}$, $z = (z_1, z_2) \in M$, where μ is the mass density, E is the Young's modulus, Δ is the two-dimensional Laplace operator, and M is a two-dimensional spatial domain with a piecewise smooth boundary. The port-Hamiltonian formulation of the vibrating string in the smooth scenario was presented in [39].

The energy variables are the 2-dimensional kinetic momentum p, and the 1-form elastic strain ϵ. The *co*-energy variables are the 0-form velocity v and the 1-form stress σ. The energy density in terms of the co-energy variables is

$$\mathsf{h} = \frac{1}{2} \left(\mu\, v \wedge *v + E\, \epsilon \wedge *\epsilon \right),$$

while the Hamiltonian is

$$H = \int_M \mathsf{h} = \frac{1}{2} \left(\mu \|v\|^2_{L^2\Omega^0} + E \|\epsilon\|^2_{L^2\Omega^1} \right).$$

The port-Hamiltonian systems is

$$\begin{aligned} \begin{pmatrix} \frac{\partial v}{\partial t} \\ \frac{\partial \epsilon}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & -\delta \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} \delta_v H \\ \delta_\epsilon H \end{pmatrix} = \begin{pmatrix} \delta\epsilon \\ \mathrm{d}v \end{pmatrix} \\ \begin{pmatrix} e_b \\ f_b \end{pmatrix} &= \begin{pmatrix} \mathrm{tr} & 0 \\ 0 & \mathrm{tr}\, * \end{pmatrix} \begin{pmatrix} \delta_v H \\ \delta_\epsilon H \end{pmatrix} = \begin{pmatrix} \mathrm{tr}\, v & 0 \\ 0 & \mathrm{tr}\, *\epsilon \end{pmatrix}, \end{aligned} \tag{2.3.32}$$

where the state variables are $v \in H\Omega^0(M)$ and $\epsilon \in H^1\Omega^1(M)$, while the boundary port-variables are $e_b \in H^{-1/2}\Omega^0(\partial M)$ and $f_b \in H^{1/2}\Omega^1(\partial M)$.

2.3.5 Composition of Stokes-Dirac Structures

In order to relate the results of Theorem 2.3.3 to the composition of the two Stokes-Dirac structures, let $X^j_{p,q} = L^2\Omega^{k-1}(M_j) \oplus L^2\Omega^k(M_j)$, $U^j_b = H^{-1/2}\Omega^{k-1}(\Gamma_j)$, and $Y^j_b = H^{1/2}\Omega^{n-k}(\Gamma_j)$. The boundary operators G^{AB} and K^{AB} are given as

$$\begin{aligned} G^{AB} &= \begin{pmatrix} \mathrm{tr}_{\Gamma_A} & 0 & 0 & 0 \\ 0 & 0 & \mathrm{tr}_{\Gamma_B} & 0 \end{pmatrix} \\ K^{AB} &= \begin{pmatrix} 0 & \mathrm{tr}_{\Gamma_A} * & 0 & 0 \\ 0 & 0 & 0 & \mathrm{tr}_{\Gamma_B} * \end{pmatrix}. \end{aligned} \tag{2.3.33}$$

The internal operator L^{AB} is biven by

$$L^{AB} = \begin{pmatrix} 0 & -\delta & 0 & 0 \\ \mathrm{d} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\delta \\ 0 & 0 & \mathrm{d} & 0 \end{pmatrix}. \tag{2.3.34}$$

The consequences of Theorem 2.3.3 are summarized by the following statement.

Corollary 2.3.6. *The boundary composition of the two Stokes-Dirac structures $\mathcal{D}^A$ and $\mathcal{D}^B$ is a Stokes-Dirac structure*

$$\mathcal{D}^A \circ \mathcal{D}^B = \left(\begin{array}{cccc} 0 & -\delta & 0 & 0 \\ \mathrm{d} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\delta \\ 0 & 0 & \mathrm{d} & 0 \\ \hline 0 & \mathrm{tr}_{\Gamma_A} * & 0 & 0 \\ 0 & 0 & 0 & \mathrm{tr}_{\Gamma_B} * \\ \hline \mathsf{id}_{L^2\Omega^{k-1}(M_A)} & 0 & 0 & 0 \\ 0 & \mathsf{id}_{L^2\Omega^k(M_A)} & 0 & 0 \\ 0 & 0 & \mathsf{id}_{L^2\Omega^{k-1}(M_B)} & 0 \\ 0 & 0 & 0 & \mathsf{id}_{L^2\Omega^k(M_B)} \\ \hline \mathrm{tr}_{\Gamma_A} & 0 & 0 & 0 \\ 0 & 0 & \mathrm{tr}_{\Gamma_B} & 0 \end{array} \right) \mathrm{dom}\, \Xi^{AB},$$

where

$$\operatorname{dom}\Xi^{AB} = \left\{ (e_p^A, e_q^A, e_p^B, e_q^B) \middle| (e_p^A, e_q^A, e_p^B, e_q^B) \in X_{p,q}^A \oplus X_{p,q}^B \right.$$
$$\left. \text{such that } \operatorname{tr}\Gamma * e_q^A + \operatorname{tr}\Gamma * e_q^B = 0 \text{ and } \operatorname{tr}\Gamma e_p^A = \operatorname{tr}\Gamma e_p^B \right\}$$

and the power product (2.3.5) induced by the unitary operator

$$r_{\mathcal{E},\mathcal{F}} = \operatorname{diag}(\mathsf{id}_{X_{p,q}^A}, \mathsf{id}_{X_{p,q}^B}, -\bar{*}_{U_b^A, Y_b^A}, -\bar{*}_{U_b^B, Y_b^B}).$$

2.4 Port-Hamiltonian Systems on Jets

So far we were looking at the formulation of port-Hamiltonian systems with respect to Dirac structures. A different, but related, approach to port-Hamiltonian systems is a field theoretic approach. Studying distributed-parameter port-Hamiltonian systems as classical field theories can be quite naturally conducted by employing the geometry of fiber bundles. This approach is the running topic of this section and will be revisited in Chapter 5.

Throughout, we closely follow [103, 104] in both the content and notation. Much more on jet bundles can be found in [94, 125], while a comprehensive treatment of port-Hamiltonian systems on jets is given in [116].

2.4.1 Preliminaries

We begin by considering the bundle $\pi : \mathcal{X} \to M$, $(\xi^A, x^\alpha) \to (\xi^A)$, where x are the dependent and ξ the independent coordinates for M. The first jet manifold $J^1(\mathcal{X})$ possesses the coordinates $(\xi^A, x^\alpha, x_A^\alpha)$, where the capital Latin indices A, B are used for the smooth n-dimensional manifold M (independent coordinates) and x_A^α denote derivative coordinates of first order (derivatives of the dependent coordinates with respect to the independent ones). The jet structure also induces the so-called total derivative

$$d_A = \partial_A + x_A^\alpha \partial_\alpha + x_{AB}^\alpha \partial_\alpha^B$$

acting on elements including first order derivatives and x_{AB}^α correspond to derivative coordinates of second order living in the second jet manifold $J^2(\mathcal{X})$. It is possible, but we will not take higher order jets and derivatives into account.

In the sequel we will pay a special attention to densities of the form $\mathfrak{H} = \mathcal{H}\mathrm{d}\xi$ for $\mathcal{H} \in C^\infty(J^1(\mathcal{X}))$, where $\mathrm{d}\xi$ denotes the volume element on

the manifold M, i.e. $\mathrm{d}\xi = \mathrm{d}\xi^1 \wedge \ldots \wedge \mathrm{d}\xi^n$. The integrated quantity of $\mathcal{H}$ is $H = \int_M \mathfrak{H}$, where the map $x = \Phi(\xi)$ leading to $x_A = \partial_A \Phi(\xi)$ needs to be specified in order to evaluate the integral.

The bundle structure $\pi : \mathcal{X} \to M$ induces the space $\bigwedge_1^n(\mathcal{X})$

$$\bigwedge\nolimits_1^n(\mathcal{X}) \quad = \quad T^*\mathcal{X} \wedge \bigwedge\nolimits^n(T^*M)\,,$$

where $\bigwedge^n(T^*M)$ is the k-fold exterior product of T^*M. The space of sections of $\bigwedge^n(T^*M)$ is the module of k-forms $\Omega^k(M)$. The coordinate representation of a typical element ω in $\bigwedge^n(T^*M)$ is $\omega = \omega_\alpha \mathrm{d}x^\alpha \wedge \mathrm{d}\xi$. It is worth pointing out that the functions ω_α may depend on derivative coordinates, however, to simplify the notation we will not explicitly indicate pull backs, that is, it should be clear from the context which order of derivative is included in the differential form. For instance, if $\omega_\alpha \in J^1(\mathcal{X})$ then $\omega \in (\pi_0^1)^* \bigwedge_1^n(\mathcal{X})$ with $\pi_0^1 : J^1(\mathcal{X}) \to \mathcal{X}$, but for simplicity we suppress the pull back and write $\omega \in \bigwedge_1^n(\mathcal{X})$.

An important object is the horizontal exterior derivative d_h given as $\mathrm{d}_h(\Phi) = \mathrm{d}\xi^A \wedge d_A(\Phi)$ when it acts on a differential form Φ, where $d_A(\Phi)$ denotes the Lie-derivative of Φ with respect to d_A. To understand the relation between the operators d and d_h and Stokes' theorem, consider a bundle $\pi : \mathcal{X} \to M$ and its m-th order jet manifold $J^m(\mathcal{X})$ as well as the bundle $\pi_0^m : J^m(\mathcal{X}) \to \mathcal{X}$ together with a section $\Phi : M \to \mathcal{X}$, that is $x = \Phi(\xi)$.

The exterior derivative d is related to the horizontal derivative d_h through

$$\left(j^{m+1}\Phi\right)^* \left(\mathrm{d}_h\left(\omega\right)\right) = \mathrm{d}\left(\left(j^m\Phi\right)^*\left(\omega\right)\right) \tag{2.4.1}$$

for a form ω living on $J^m(\mathcal{X})$. Roughly speaking, the pull back $\left(j^m\Phi\right)^*(\omega)$ denotes $\omega \circ (j^m\Phi)$ for $j^m\Phi$ corresponding to the m-th order jet-lift of the section Φ.

Integrating $j^{m+1}\left(\Phi\right)^*\left(\mathrm{d}_h\omega\right)$ over the oriented compact manifold M results in

$$\int_M j^{m+1}\left(\Phi\right)^*\left(\mathrm{d}_h\omega\right) = \int_M \mathrm{d}\left(j^m\left(\Phi\right)^*\left(\omega\right)\right) = \int_{\partial M} j^m\left(\Phi\right)^*\left(\omega\right)$$

for any $\omega \in (\pi_0^m)^*(\bigwedge^{m-1}(\mathcal{X}))$, which is nothing else than Stokes' theorem on jet bundles.

2.4.2 Hamiltonian Structure

Let us consider a vertical vector field $v : \mathcal{X} \to V(\mathcal{X})$ locally given as $v = v^\alpha \partial_\alpha$, where v^α may depend on derivative coordinates, together with its first jet-prolongation $j^1(v)$ given by

$$j^1(v) \quad = \quad v^\alpha \partial_\alpha + d_A(v^\alpha)\partial_\alpha^A.$$

Then we compute the Lie-derivative of the density $\mathfrak{F}$ as it has been defined before with respect to the vector field $j^1(v)$ and we obtain the important relation

$$\begin{aligned} j^1(v)(\mathcal{H}\mathrm{d}\xi) &= \left(v^\alpha(\partial_\alpha\mathcal{H} - d_A\partial^A_\alpha\mathcal{H}) + d_A(v^\alpha\partial^A_\alpha\mathcal{H})\right)\mathrm{d}\xi \\ &= \left(v^\alpha\delta_\alpha\mathcal{H} + d_A(v^\alpha\partial^A_\alpha\mathcal{H})\right)\mathrm{d}\xi. \end{aligned} \tag{2.4.2}$$

The *Euler-Lagrange operator* δ

$$\delta : J^2(\mathcal{X}) \to \textstyle\bigwedge^n_1(\mathcal{X}) \tag{2.4.3}$$

comes into play, whose coordinate expressions involves the variational derivative δ_α, which acts on $\mathcal{H}$ as

$$\delta_\alpha\mathcal{H} = \partial_\alpha\mathcal{H} - d_A\partial^A_\alpha\mathcal{H}.$$

Applying the Stokes theorem to (2.4.2) yields

$$\begin{aligned} \int_M j^1(v)(\mathcal{H}\mathrm{d}\xi) &= \int_M v^\alpha\left(\delta_\alpha\mathcal{H}\right)\mathrm{d}\xi + \int_{\partial M} v^\alpha\left(\partial^A_\alpha\mathcal{H}\right)\mathrm{d}\xi_A \\ &= \int_M v\rfloor\delta\mathfrak{H} + \int_{\partial M} v\rfloor\delta^\partial\mathfrak{H}, \end{aligned} \tag{2.4.4}$$

where $\mathrm{d}\xi_A = \partial_A\rfloor\mathrm{d}\xi$, with $\rfloor$ being a contraction operator, and the boundary operator given by

$$\delta^\partial\mathfrak{H} = \partial^A_\alpha\mathcal{H}\,\mathrm{d}x^\alpha\wedge\mathrm{d}\xi_A.$$

The relation (2.4.4) is of a key interest since it provides a natural decomposition of the expression $\int_M j^1(v)(\mathcal{H}\mathrm{d}\xi)$ into a term on the domain M and a term on the boundary ∂M.

2.4.3 Port-Hamiltonian Representation

In order to introduce a port-Hamiltonian system on a bundle $\mathcal{X}\to M$, we start with a Hamiltonian density function of first order $\mathcal{H}\in C^\infty(J^1(\mathcal{X}))$ and the resulting Hamiltonian $\mathfrak{H} = \mathcal{H}\mathrm{d}\xi$.

Consider the skew-symmetric mapping

$$J : \textstyle\bigwedge^n_1 \to V(\mathcal{X}),$$

which satisfies

$$J(\omega_1)\rfloor(\omega_2) + J(\omega_2)\rfloor(\omega_1) = 0 \quad \text{for any } \omega_1,\omega_2\in\textstyle\bigwedge^n_1. \tag{2.4.5}$$

For the purposes of dealing with open systems, introduce the input and the output bundles as $U \to \mathcal{X}$ and $Y \to \mathcal{X}$. Given a map $G : U \to V(\mathcal{X})$, its adjoint $G^* : \bigwedge_1^n \to Y$ satisfies

$$(u \rfloor G) \rfloor \omega = u \rfloor (G^* \rfloor \omega). \tag{2.4.6}$$

This allows us to define *Hamiltonian dynamics*

$$\begin{array}{rcl} \dot{x} & = & J(\delta\mathfrak{H}) + u \rfloor G \\ y & = & G^* \rfloor \delta\mathfrak{H}, \end{array} \tag{2.4.7}$$

together with appropriate boundary conditions.

Since in local coordinates $\delta\mathfrak{H}$ is represented by

$$\delta\mathfrak{H} : (\delta_\alpha \mathcal{H}) \to (\delta_\alpha \mathcal{H}) \mathrm{d}x^\alpha \wedge \mathrm{d}\xi, \quad \text{where} \quad \delta_\alpha = \partial_\alpha - d_A \partial^A_\alpha \,, \tag{2.4.8}$$

if the mapping J is linear, the local coordinate representation of (2.4.7) is

$$\begin{array}{rcl} \dot{x}^\alpha & = & J^{\alpha\beta}(\delta_\beta \mathcal{H}) + G^\alpha_i u^i \\ y_i & = & G^\alpha_i \delta_\alpha \mathcal{H}. \end{array} \tag{2.4.9}$$

The time derivative of the Hamiltonian is

$$\begin{array}{rcl} \dot{H} & = & \displaystyle\int_M J(\delta\mathfrak{H}) \rfloor \delta\mathfrak{H} + \int_M (u \rfloor G) \rfloor \delta\mathfrak{H} + \int_{\partial M} \dot{x} \rfloor \delta^\partial \mathfrak{H} \\ & = & \displaystyle\int_M u \rfloor y + \int_{\partial M} \dot{x} \rfloor \delta^\partial \mathfrak{H} \,, \end{array} \tag{2.4.10}$$

which reflects the power balance, since the total change of the functional H along solutions of (2.4.7) depends on collocation on the domain and an expression corresponding to a boundary port (if it exists) depending on the boundary conditions, see [116, 103, 104].

2.4.4 Vibrating String

As a recurring example of this thesis, consider an elastic string of length l, elasticity modulus T, and mass density μ, subject to traction forces at its ends. The underlying manifold is the segment $M = [0, l] \subset \mathbb{R}$. The independent coordinate is the spatial coordinate ξ and the dependent coordinates are the deflection u and the temporal momentum p. This leads to the following bundle $\mathcal{X} \to M$, $(\xi, u, p) \to \xi$. The first jet manifold $J^1(\mathcal{X})$ additionally includes the derivative coordinates u_ξ and p_ξ. The boundary ∂M consists of just two points

only, namely $\xi = 0$ and $\xi = l$. The set of partial differential equations that describe the system is

$$\begin{array}{rcl} \dot{u} & = & \frac{p}{\mu} \\ \dot{p} & = & d_\xi(Tu_\xi) \end{array} \tag{2.4.11}$$

together with additional boundary conditions. To rewrite this system in a Hamiltonian fashion consider the Hamiltonian density $\mathfrak{H} = \mathcal{H}\mathrm{d}\xi$ with

$$\mathcal{H} = \frac{1}{2\rho}p^2 + \frac{1}{2}Tu_\xi^2. \tag{2.4.12}$$

The total Hamiltonian is $H = \int_0^L \mathcal{H}\mathrm{d}\xi$. To obtain partial differential equations in the form as in (2.4.7) we set G to zero. Then

$$\begin{pmatrix} \dot{u} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \delta_u\mathcal{H} \\ \delta_p\mathcal{H} \end{pmatrix} = J(\delta\mathfrak{H}),$$

where $x = (u, p)$ and the variational derivatives are

$$\delta_u\mathcal{H} = \left(\partial_u - d_\xi\partial_u^\xi\right)\mathcal{H} = -d_\xi(Tu_\xi)$$

and

$$\delta_p\mathcal{H} = \left(\partial_p - d_\xi\partial_p^\xi\right)\mathcal{H} = \frac{p}{\mu}.$$

Evaluating (2.4.10) gives

$$\dot{H} = \int_{\partial M} \dot{x}\rfloor\delta^\partial\mathfrak{H} = \dot{u}Tu_\xi|_0^l\ . \tag{2.4.13}$$

Let $f_b = \mathrm{tr}(\frac{p}{\mu}) \in \mathcal{F}_b$ be the boundary flow and $e_b = \mathrm{tr}(Tu_\xi) \in \mathcal{F}_b^*$ be the boundary effort variable. The time derivative of the Hamiltonian in (2.4.13) now can be rewritten as

$$\dot{H} = \int_{\partial M} e_b f_b = e_b(l)f_b(l) - e_b(0)f_b(0)$$

expressing the fundamental property of all port-Hamiltonian systems.

The correlation between formulation (2.4.7) and Stokes-Dirac structures will be studied in Chapter 5.

3
Structure-Preserving Discretization

> A common way to generate questions (not only) in geometry is to confront properties of objects specific to different categories: what is a possible topology (e.g. homology) of a manifold with a given type of curvature? ... These seduce us by simplicity and apparent naturality, sometimes leading to new ideas and structures but often the mirage of naturality lures us into featureless desert with no clear perspective where the solution, even if found, does not quench our thirst for structural mathematics.
>
> – Misha Gromov, *Spaces and questions*

In this chapter I propose a *geometric* framework for structure-preserving discretization of distributed-parameter port-Hamiltonian systems. The approach to time-continuous spatially-discrete port-Hamiltonian theory is based on discrete exterior geometry and as such proceeds *ab initio* by mirroring the continuous setting. The theory is not merely tied to the goal of discretization but rather aims to offer a sound and consistent framework for defining port-Hamiltonian dynamics on a discrete manifold which is usually, but not necessarily, obtained by discretization of a smooth Riemannian manifold.

In order to make this chapter as self-contained as possible for a variety of readers, I present a brief overview of the discrete exterior geometry needed to define a discretized Stokes-Dirac structure and port-Hamiltonian dynamics. The third section is a brief summary of the essential definitions and results in discrete exterior calculus as developed in [26, 27, 49]. The contribution of this thesis in this regard is a proper treatment of the boundary of the dual cell complex. Namely, in order to allow the inclusion of nonzero boundary conditions on the dual cell complex, I offer a definition of the dual boundary operator that differs from the standard one. Such a construction leads to a discrete analogue

of the integration by parts formula, which is a crucial ingredient in establishing a discrete Stokes-Dirac structure on a primal simplicial complex and its circumcentric dual. The main result is presented in Section 3.2, where I introduce the notion of simplicial Dirac structures on a primal-dual cell complex, and in the following section define port-Hamiltonian systems with respect to these structures. Finally, I demonstrate how the simplicial Dirac structures relate to some spatially discretized distributed-parameter systems with boundary variables: Maxwell's equations on a bounded domain, a two-dimensional wave equation, and the telegraph equations.

3.1 Fundaments of Discrete Exterior Calculus

The discrete manifolds we employ are oriented manifold-like simplicial complexes and their circumcentric duals. Typically, these manifolds are simplicial approximations of smooth manifolds. Familiar examples are meshes of triangles embedded in $\mathbb{R}^3$ and tetrahedra obtained by tetrahedrization of a 3-dimensional manifold. There are many ways to obtain such complexes; however, we do not address the issue of discretization and embedding.

As said, we proceed *ab initio* and mostly our treatment is purely formal, that is without proofs that the discrete objects converge to the continuous ones, though we briefly address the issue of convergence in Chapter 4 (see Section 4.4). By construction of discrete exterior calculus, a number of important geometric structures are preserved and propositions like Stokes theorem are true by definition. The basic building blocks of discrete exterior geometry are discrete chains and cochains, and their geometric duals. The former are simplices and the latter are discrete differential forms related one to another by bilinear pairing that can be understood as the evaluation of a cochain on an appropriate simplex, and as such parallels integration in the continuous setting.

In discrete exterior calculus, a *dual mesh* is instrumental for defining the diagonal Hodge star. In the thesis at hand, the geometric duality is a crucial ingredient in establishing a bijective relationship between the flow and effort spaces, as well as for the construction of nondegenerate discrete analogues of the bilinear form (2.2.1).

This section, with some modification concerning the treatment of the boundary of the dual cell complex, is a brief summary of the essential definitions and results in discrete exterior calculus as developed in [26, 27, 49]. As therein, first we define discrete differential forms, the discrete exterior derivative, the codifferential operator, the Hodge star, and the discrete wedge prod-

uct. For more information on the construction of the other discrete objects such as vector fields, a discrete Lie derivative, and discrete musical operators, we refer the reader to [49]. Construction of all these discrete objects is in a way simpler than their continuous counterparts since we require only a local metric; ergo the machinery of the Riemannian geometry is not demanded. With the exception of the treatment of the notions related to the boundary of the dual cell complex, a good part of this section is a recollection of the basic concepts and results of algebraic topology [46, 73].

3.1.1 Simplicial Complexes and Their Circumcentric Duals

Definition 3.1.1. *A k-**simplex** σ^k is the convex span of $k+1$ geometrically independent points,*

$$\sigma^k = [v_0, v_1, \ldots, v_k] := \left\{ \sum_{i=0}^{k} \alpha^i v_i \,\middle|\, \alpha^i \geq 0, \sum_{i=0}^{n} \alpha^i = 1 \right\}.$$

The points $v_0, \ldots, v_k$ are called the vertices of the simplex, and the number k is called the dimension of the simplex. Any simplex spanned by a (proper) subset of $\{v_0, \ldots, v_k\}$ is called a (proper) face of σ^k. If σ^l is a proper face of σ^k, we denote this by $\sigma^l \prec \sigma^k$.

As an illustration, consider four non-collinear points v_0, v_1, v_2, and v_3 in $\mathbb{R}^3$. Each of these points individually is a 0-simplex with an orientation dictated by the choice of a sign. An example of a 1-simplex is a line segment $[v_0, v_1]$ oriented from v_0 to v_1. The triangle $[v_0, v_1, v_2]$ is an example of a 2-simplex oriented in counterclockwise direction. Finally, the tetrahedron $[v_0, v_1, v_2, v_3]$ is a 3-simplex.

Definition 3.1.2. *A **simplicial complex** K in $\mathbb{R}^N$ is a collection of simplices in $\mathbb{R}^N$, such that:*

(1) *Every face of a simplex of K is in K.*

(2) *The intersection of any two simplices of K is a face of each of them.*

The dimension n of the highest dimension simplex in K is the dimension of K.

The above given definition of a simplicial complex is more general than needed for the purposes of exterior calculus. Since the discrete theory employed in this thesis mirrors the continuous framework, we restrict our considerations to *manifold-like simplicial complexes* [49].

Definition 3.1.3. *A simplicial complex K of dimension n is a* ***manifold-like simplicial complex*** *if the underlying space is a polytope $|K|$. In such a complex all simplices of dimension $k = 0, \ldots, n-1$ must be a face of some simplex of dimension n in the complex.*

Introducing these simplicial meshes has an added advantage of allowing a simple and intuitive definition of orientability of simplicial complexes [49].

Definition 3.1.4. *An n-dimensional simplicial complex K is an oriented manifold-like simplicial complex if the n-simplices that share a common $(n-1)$-face have the same orientation and all the simplices of lower dimensions are individually oriented.*

Henceforth in this chapter, we shall work with manifold-like simplicial complexes. When no confusion can arise, we address these objects simply as simplicial complexes.

An essential constituent of discrete exterior calculus is the dual complex of a manifold-like simplicial complex. The most popular notions of duality are barycentric and circumcentric, also known as Voronoi, duality. Following the standard approach of discrete exterior calculus, in this chapter we employ the latter.

The circumcenter of a k-simplex σ^k is given by the center of the k-circumsphere, which is the unique k-sphere that has all $k+1$ vertices of σ^k on its surface. That is, the circumcenter is the unique point in the k-dimensional affine space that contains the k-simplex that is equidistant from all the $k+1$ vertices of the simplex. We denote the circumcenter of a simplex σ^k by $c(\sigma^k)$.

If the circumcenter of a simplex lies in its interior we call it a ***well-centered simplex***. For instance, a triangle with all acute angles is a well-centered 2-simplex. A simplicial complex K whose all simplices of all dimensions are well-centered is called a well-centered simplicial complex and its dual obtained by circumcentric subdivision is also a simplicial complex denoted by $\operatorname{csd} K$ and its elements by $\hat{\sigma}^0, \ldots, \hat{\sigma}^n$. Throughout this thesis, we adopt the convention that all symbols related to the dual (simplicial and cell) complex are labeled by a caret. The underlying spaces $|K|$ and $|\operatorname{csd} K|$ are the same. The simplicial complex $\operatorname{csd} K$ consists of all simplices of the form $[c(\sigma_1), \ldots, c(\sigma_k)]$ for $k = 1, \ldots, n$, where $\sigma_1 \prec \sigma_2 \prec \ldots \prec \sigma_k$, meaning σ_i is a proper face of σ_j for all $i < j$.

A circumcentric dual cell complex (block complex in the terminology of [73]) is obtained by aggregation of certain simplices of $\operatorname{csd} K$. Let K be a well-centered simplicial complex of dimension n and let σ^k be one of its simplices. By $D(\sigma^p)$ we denote the union of all open simplices of $\operatorname{csd} K$ of which $c(\sigma^k)$

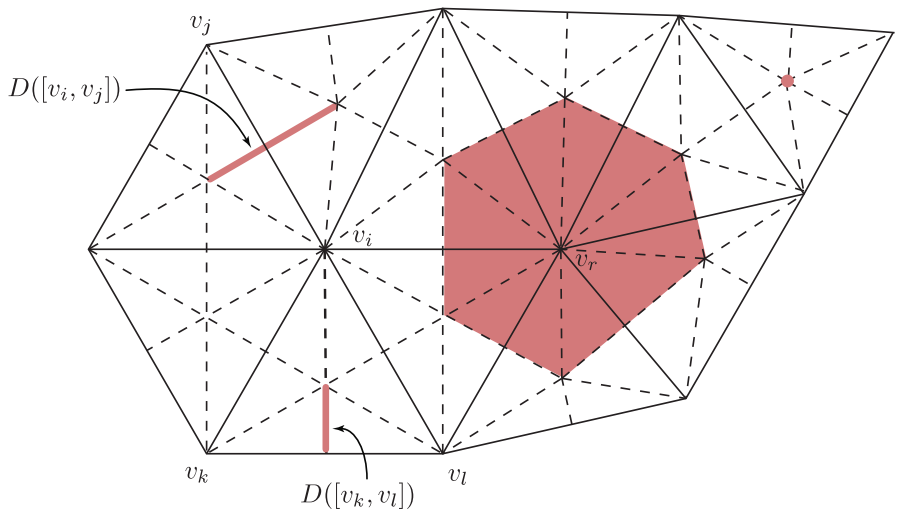


Figure 3.1: A 2-dimensional simplicial complex K subdivided into the circumcentric simplicial complex $\operatorname{csd} K$ indicated by dotted lines. The dual cells displayed are shaded.

is the final vertex; this cell is the dual cell to σ^k. The closure of the dual cell of σ^k is $\bar{D}(\sigma^k)$. The collection of all dual cells is a cell complex denoted by $D(K)$ with closure $\bar{D}(K)$.

To illustrate the duality, consider the 2-dimensional simplicial complex pictured in Figure 3.1. The dual cell of the vertex v_r is the topological interior of the Voronoi region around it as shown shaded in the figure. This dual cell is comprised of the vertex v_r, the interior of the open edges emanating from v_r, and interiors of the all dual simplices containing v_r. The dual cell of any 2-simplex consists of its circumcenter alone. The dual cell of an edge consists of its circumcenter and two open edges joining this circumcenter to the circumcenters of two triangles having the primal edge as a face. The dual of a boundary edge has only one half-edge since there is only one triangle adjacent to that boundary edge. Note that if the complex is not flat, then the dual edge will not be a straight line.

Remark 3.1.1. *A triangulation of a compact n-dimensional Riemannian manifold M results in an n-dimensional simplicial complex K. Intuitively, the simplices are glued to the manifold M in such a way that they form a 'curved' manifold-like simplicial complex. It is worth noticing that in practical applications, the smooth manifold sometimes is unknown and can only be sam-*

pled by physical measurements. In such situations, it makes sense to model the spatial domain as inherently discrete. This is where discrete port-Hamiltonian theory in the framework of discrete exterior calculus stands in its own right.

3.1.2 Chains and Cochains

The discrete analogue of a smooth k-form is a k-cochain, a linear function, on k-chains representing a formal sum of simplices. In the discrete theory, the role of integration is replaced by (simple) evaluation of a cochain (a discrete form) on a k-chain. The discrete exterior derivative is defined by duality to the boundary operator, rendering the Stokes theorem true by definition. Parallel to the smooth case, the discrete exterior wedge product pairs lower degree forms into a higher degree one.

Definition 3.1.5. *Let K be a simplicial complex. We denote the free Abelian group generated by a basis consisting of oriented k-simplices by $C_k(K;\mathbb{Z})$. This is the space of finite formal sums of the k-simplices with coefficients in $\mathbb{Z}$. Elements of $C_k(K;\mathbb{Z})$ are called k-chains.*

Definition 3.1.6. *A primal discrete k-form α is a homomorphism from the chain group $C_k(K;\mathbb{Z})$ to the additive group $\mathbb{R}$. Thus, a discrete k-form is an element of* $\mathrm{Hom}(C_k(K),\mathbb{R})$*, the space of cochains. This space becomes an Abelian group if we add two homomorphisms by adding their values in $\mathbb{R}$. The standard notation for* $\mathrm{Hom}(C_k(K),\mathbb{R})$ *in algebraic topology is $C^k(K;\mathbb{R})$; however, like in [26, 27, 49] we shall throughout employ the notation $\Omega_d^k(K)$ for this space as a reminder that this is the space of discrete k-forms on the simplicial complex K. Thus,*

$$\Omega_d^k(K) := C^k(K;\mathbb{R}) = \mathrm{Hom}(C_k(K),\mathbb{R})\,.$$

Given a k-chain $\sum_i a_i c_i^k$, $a_i \in \mathbb{Z}$, and a discrete k-form α, we have

$$\alpha\left(\sum_i a_i c_i^k\right) = \sum_i a_i \alpha(c_i^k)\,,$$

and for two discrete k-forms $\alpha, \beta \in \Omega_d^k(K)$ and a k-chain $c \in C_k(K;\mathbb{Z})$,

$$(\alpha+\beta)(c) = \alpha(c) + \beta(c)\,.$$

The natural pairing of a k-form α and a k-chain c is defined as the bilinear pairing $\langle \alpha, c\rangle = \alpha(c)$.

As previously pointed out, a differential k-form $\alpha^k \in \Omega_d^k(K)$ can be thought of as a linear functional that assigns a real number to each oriented cell $\sigma^k \in K$. In order to understand the process of discretization of the continuous problem consider a smooth k-form $f \in \Omega^k(|K|)$. The discrete counterpart of f on a k-simplex $\sigma^k \in K$ is a discrete form α^k defined as $\alpha^k(\sigma^k) := \int_{\sigma^k} f$.

Definition 3.1.7. *The **boundary operator** $\partial_k : C_k(K;\mathbb{Z}) \to C_{k-1}(K;\mathbb{Z})$ is the homomorphism defined by its action on a simplex $\sigma^k = [v_0, \ldots, v_k]$ as*

$$\partial_k \sigma^k = \partial_k([v_0, \ldots, v_k]) = \sum_{i=0}^{k} (-1)^i [v_0, \ldots, \hat{v}_i, \ldots, v_k] \,,$$

where $[v_0, \ldots, \hat{v}_i, \ldots, v_k]$ is the $(k-1)$-simplex obtained by omitting the vertex v_i. Note that $\partial_k \circ \partial_{k+1} = 0$.

Definition 3.1.8. *On a simplicial complex of dimension n, a **chain complex** is the collection of chain groups and homomorphisms ∂_k, satisfying*

$$0 \longrightarrow C_n(K) \xrightarrow{\partial_n} C_{n-1} \xrightarrow{\partial_{n-1}} \cdots \xrightarrow{\partial_{k+1}} C_k(K) \xrightarrow{\partial_k} \cdots \xrightarrow{\partial_1} C_0(K) \xrightarrow{\partial_0} 0 \,,$$

and $\partial_k \circ \partial_{k+1} = 0$.

For instance, given an oriented triangle $[v_0, v_1, v_2]$ the boundary, by the above definition, is the chain $[v_0, v_1] + [v_1, v_2] - [v_0, v_2]$, which is composed of the 3 boundary edges of the triangle.

Definition 3.1.9. *The **discrete exterior derivative** $\mathbf{d} : \Omega_d^k(K) \to \Omega_d^{k+1}(K)$ is defined by duality to the boundary operator $\partial_{k+1} : C_{k+1}(K;\mathbb{Z}) \to C_k(K;\mathbb{Z})$, with respect to the natural pairing between discrete forms and chains. For a discrete form $\alpha^k \in \Omega_d^k(K)$ and a chain $c_{k+1} \in C_{k+1}(K;\mathbb{Z})$ we define $\mathbf{d}$ by*

$$\langle \mathbf{d}\alpha^k, c_{k+1} \rangle = \langle \alpha^k, \partial_{k+1} c_{k+1} \rangle \,.$$

The discrete exterior derivative is the coboundary operator from algebraic topology [73] and as such it induces the cochain complex

$$0 \longleftarrow \Omega_d^n(K) \xleftarrow{\mathbf{d}} \Omega_d^{n-1} \xleftarrow{\mathbf{d}} \cdots \xleftarrow{\mathbf{d}} \Omega_d^0(K) \longleftarrow 0 \,,$$

where $\mathbf{d} \circ \mathbf{d} = 0$.

Such as in the continuous theory, we drop the index of the boundary operator ∂_k when its dimension is clear from the context. The discrete exterior derivative $\mathbf{d}$ has been constructed in such a manner that the Stokes theorem

is satisfied by definition. This means, given a $(k+1)$-chain c and a discrete k-form α, the ***discrete Stokes theorem*** states that

$$\langle \mathbf{d}\alpha, c\rangle = \langle \alpha, \partial c\rangle \,.$$

Consider a k-chain $\sum_i a_i c_i$, $a_i \in \mathbb{Z}$, $c_i \in C_k(K;\mathbb{Z})$, and $(k-1)$-form $\alpha \in \Omega_d^{k-1}(K;\mathbb{Z})$. By linearity of the chain-cochain pairing, the discrete Stokes theorem can be stated as

$$\left\langle \mathbf{d}\alpha, \sum_i a_i c_i \right\rangle = \left\langle \alpha, \partial\left(\sum_i a_i c_i\right)\right\rangle = \left\langle \alpha, \sum_i a_i \partial c_i \right\rangle = \sum_i a_i \left\langle \alpha, \partial c_i\right\rangle \,.$$

As in the continuous setting, the discrete wedge product pairs two discrete differential forms by building a higher degree form. The primal-primal wedge product inherits some important properties of the cup product such as the bilinearity, anticommutativity and naturality under pull-back [26, 49]; however, it is in general non-associative and degenerate, and thus unsuitable for construction of canonical pairing between the flow and effort space. For a definition of nondegenerate pairing between the flow and effort discrete forms we shall use a primal-dual wedge product as will be defined in the subsequent section.

3.1.3 Metric-Dependent Part of Discrete Exterior Calculus

A cellular chain group associated with the dual cell complex $D(K)$, in [73] denoted by $D_p(K)$, is the group of formal sums of cells with integer coefficients. Since in $D(K)$ the information of dual simplices is lost, to retain the bookkeeping information Hirani in [49] introduces a duality operator which takes values in the domain group $C_p(\operatorname{csd} K;\mathbb{Z})$. As will be clear from the subsequent section, this bookkeeping is not indispensable for the formulation of the Dirac structure on a simplicial complex; nevertheless, since the information of dual simplices might be needed in defining dynamics, we also employ this construction.

In order to explicitly construct the duality on the boundary, in the next definition we introduce the boundary star operator. Shortly afterward we shall explain the rational behind this construction.

Definition 3.1.10. *Let K be a well-centered simplicial complex of dimension n. The interior circumcentric duality operator* $\star_{\mathrm{i}} : C_k(K;\mathbb{Z}) \to C_{n-k}(\operatorname{csd} K;\mathbb{Z})$

$$\star_{\mathrm{i}}(\sigma^k) = \sum_{\sigma^k \prec \sigma^{k+1} \prec \cdots \prec \sigma^n} s_{\sigma^k,\ldots,\sigma^n}\left[c(\sigma^k), c(\sigma^{k+1}), \ldots, c(\sigma^n)\right] \,,$$

and the boundary star operator $\star_{\mathrm{b}} : C_k(\partial K;\mathbb{Z}) \to C_{n-1-k}(\partial(\operatorname{csd} K);\mathbb{Z})$

$$\star_{\mathrm{b}}(\sigma^k) = \sum_{\sigma^k \prec \sigma^{k+1} \prec \cdots \prec \sigma^{n-1}} s_{\sigma^k,\ldots,\sigma^{n-1}} \left[c(\sigma^k), c(\sigma^{k+1}), \ldots, c(\sigma^{n-1}) \right] ,$$

where the $s_{\sigma^k,\ldots,\sigma^n}$ *and* $s_{\sigma^k,\ldots,\sigma^{n-1}}$ *coefficients ensure that the orientation of the cell* $[c(\sigma^k), c(\sigma^{k+1}), \ldots, c(\sigma^n)]$ *and* $[c(\sigma^k), c(\sigma^{k+1}), \ldots, c(\sigma^{n-1})]$ *is consistent with the orientation of the primal simplex, and the ambient volume forms on* K *and* ∂K*, respectively.*

The subset of chains $C_p(\operatorname{csd} K;\mathbb{Z})$ that are equal to the cells of $D(K) \times D(\partial K)$ forms a subgroup of $C_p(\operatorname{csd} K;\mathbb{Z})$. We denote this subgroup of $C_p(\operatorname{csd} K;\mathbb{Z})$ by $C_p(\star K;\mathbb{Z})$, where $\star K$ is its basis set. A cell complex $\star K$ in $\mathbb{R}^N$ is a collection of cells in $\mathbb{R}^N$ such that: (1) there is a partial ordering of cells in $\star K$, $\hat{\sigma}^k \prec \hat{\sigma}^l$, which is read as $\hat{\sigma}^k$ is a face of $\hat{\sigma}^l$; (2) the intersection of any two cells in $\star K$, is either a face of each of them, or it is empty; (3) the boundary of a cell is expressed as a sum of its proper faces.

Given a simplicial well-centered complex K, we define its interior dual cell complex $\star_{\mathrm{i}} K$ (block complex in terminology of algebraic topology [73]) as the circumcentric dual restricted to $|K|$. An important property of the the Voronoi duality is that primal and dual cells are orthogonal to each other. The boundary dual cell complex $\star_{\mathrm{b}} K$ is a dual to ∂K. The dual cell complex $\star K$ is defined as $\star K = \star_{\mathrm{i}} K \times \star_{\mathrm{b}} K$. A dual mesh $\star_{\mathrm{i}} K$ is a dual to K in sense of a graph dual, and the dual of the boundary is equal to the boundary of the dual, that is $\partial(\star K) = \star(\partial K) = \star_{\mathrm{b}} K$. This construction of the dual is compatible with [120, 48] and as such is very similar to the use of the ghost cells in finite volume methods in order to account for the duality relation between the Dirichlet and the Neumann boundary conditions. Because of duality, there is a one-to-one correspondence between k-simplices of K and interior $(n-k)$-cells of $\star K$. Likewise, to every k-simplex on ∂K there is a uniquely associated $(n-1-k)$-cell on $\partial(\star K)$.

In what follows, we shall abuse notation and use the same symbol $\star$ for both the interior circumcentric and the boundary star operator. The difference, if not clear from the exposition, will be delineated by indicating that $\star\sigma^k \in \partial(\star K)$ when $\star\sigma^k$ is a dual cell on the boundary of the dual cell complex $\star K$. As sets, the set of $\bar{D}(\sigma^p)$ and $\star\sigma^p$ are equal, the only difference being in the bookkeeping, since in $\star\sigma^p$ one retains the information about the simplices it is built of.

Here we do not address the problem of the orientation of dual $\star K$, for which we direct the reader to [49]. The circumcentric dual cell complex of the 2-dimensional simplicial complex from Figure 3.1 is pictured in Figure 3.2.

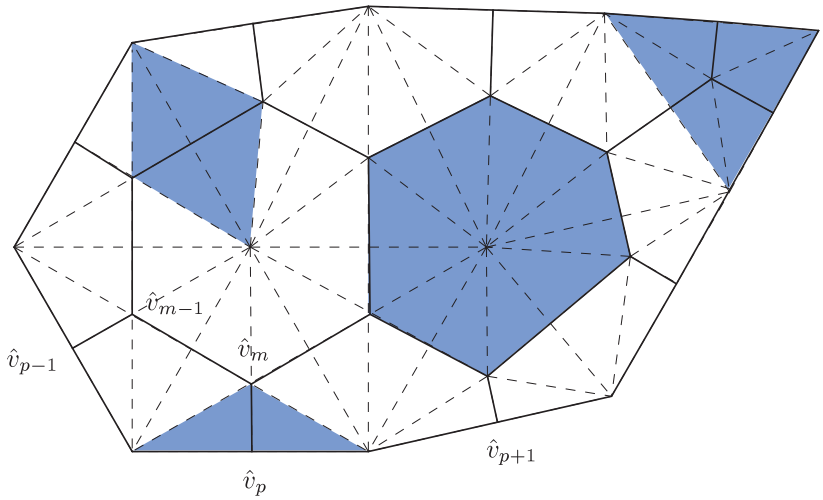


Figure 3.2: The circumcentric dual cell complex $\star K$ of the simplicial complex K given in Figure 3.1. The boundary of $\star K$ is the dual of the boundary of K. Some support volumes are shaded. For instance, the support volume of the primal vertex v_r is the area of its Voronoi region; also $V_{[v_i,v_j]} = V_{\bar{D}([v_i,v_j])}$.

An important concept in defining a wedge product between primal and dual cochains is the notion of a support volume associated with a given simplex or cell.

Definition 3.1.11. *The support volume of a simplex σ^k is an n-volume given by the convex hull of the geometric union of the simplex and its circumcentric dual. This is given by*

$$V_{\sigma^k} = \mathrm{CH}(\sigma^k, \star_{\mathrm{i}}\sigma^k) \cap |K| \,,$$

where $\mathrm{CH}(\sigma^k, \star_{\mathrm{i}}\sigma^k)$ is the n-dimensional convex hull generated by $\sigma^k \cup \star_{\mathrm{i}}\sigma^k$. The intersection with $|K|$ is necessary to ensure that the support volume does not extend beyond the polytope $|K|$ which would otherwise occur if K is non-convex. The support volume of a dual cell $\star_{\mathrm{i}}\sigma^k$ is

$$V_{\star_{\mathrm{i}}\sigma^k} = \mathrm{CH}(\star_{\mathrm{i}}\sigma^k, \star_{\mathrm{i}} \star_{\mathrm{i}} \sigma^k) \cap |K| = V_{\sigma^k} \,.$$

Everything that has been said about the primal chains and cochains can be extended to dual cells and dual cochains. We do not elaborate on this since it can be found in the literature [49, 27], however, in order to properly account for the behaviours on the boundary, we need to adapt the definition of the

boundary dual operator as presented in [49, 27]. We propose the following definition.

Definition 3.1.12. *The dual boundary operator* $\partial : C_k(\star_{\mathrm{i}} K; \mathbb{Z}) \to C_{k-1}(\star K; \mathbb{Z})$ *is a homomorphism defined by its action on a dual cell* $\hat{\sigma}^k = \star_{\mathrm{i}} \sigma^{n-k} = \star_{\mathrm{i}} [v_0, \ldots, v_{n-k}]$,

$$\partial \hat{\sigma}^k = \partial \star_{\mathrm{i}} [v_0, \ldots, v_{n-k}] = \partial_{\mathrm{i}} \star_{\mathrm{i}} [v_0, \ldots, v_{n-k}] + \partial_{\mathrm{b}} \star_{\mathrm{i}} [v_0, \ldots, v_{n-k}] ,$$

where

$$\begin{aligned} \partial_{\mathrm{i}} \star_{\mathrm{i}} [v_0, \ldots, v_{n-k}] &= \sum_{\sigma^{n-k+1} \succ \sigma^{n-k}} \star_{\mathrm{i}} (s_{\sigma^{n-k+1}} \sigma^{n-k+1}) \\ \partial_{\mathrm{b}} \star_{\mathrm{i}} [v_0, \ldots, v_{n-k}] &= \star_{\mathrm{b}} \left(s_{\sigma^{n-k}} \sigma^{n-k} \right) . \end{aligned}$$

Note that the dual boundary operator as defined in [49] is equal to ∂_{i}. Hence, the dual boundary is not the geometric boundary of a cell, because near the boundary of a manifold that would be wrong. As an example consider the complex in Figure 3.3. The dual of the vertex v_1 is the Voronoi region shown shaded. Its geometric boundary has five sides (two half primal edges and three dual edges), whereas the dual boundary according to the definition given in [49] consists of just dual edges, i.e. $[c([v_0, v_1]), c([v_0, v_1, v_2])]$, $[c([v_0, v_1, v_2]), c([v_1, v_3, v_2])]$ and $[c([v_1, v_3, v_2]), c([v_1, v_3])]$, all up to a sign depending on the chosen orientation. However, according to the above given definition, the boundary is comprised of four edges, three already given plus the boundary edge $[c([v_0, v_1]), c([v_1, v_3])]$ obtained by aggregation of the two dual simplices $[c([v_0, v_1]), v_1]$ and $[v_1, c([v_1, v_3])]$. This construction of the dual boundary ensures a natural pairing between a primal 0-form defined on v_1 and a dual 1-form on $[c([v_0, v_1]), c([v_1, v_3])]$. The offered definition of the dual boundary operator, as will be demonstrated later, is crucial for the inclusion of the boundary variables in the discrete setting.

Definition 3.1.13. *The* ***dual discrete exterior derivative*** $\mathbf{d} : \Omega_d^k(\star K) \to \Omega_d^{k+1}(\star_{\mathrm{i}} K)$ *is defined by duality to the boundary operator* $\partial : C_{k+1}(\star_{\mathrm{i}} K; \mathbb{Z}) \to C_k(K; \mathbb{Z})$. *For a dual discrete form* $\hat{\alpha}^k \in \Omega_d^k(\star K)$ *and a chain* $\hat{c}_{k+1} \in C_{k+1}(\star_{\mathrm{i}} K; \mathbb{Z})$ *we define* $\mathbf{d}$ *by*

$$\langle \mathbf{d} \hat{\alpha}^k, \hat{c}_{k+1} \rangle = \langle \hat{\alpha}^k, \partial \hat{c}_{k+1} \rangle .$$

The dual discrete exterior derivative $\mathbf{d}$ *can be decomposed into the two operators* $\mathbf{d}_{\mathrm{i}}$ *and* $\mathbf{d}_{\mathrm{b}}$, *which are respectively dual to* ∂_{i} *and* ∂_{i}, *that is*

$$\langle \mathbf{d} \hat{\alpha}^k, \hat{c}_{k+1} \rangle = \langle \mathbf{d}_{\mathrm{i}} \hat{\alpha}^k, \hat{c}_{k+1} \rangle + \langle \mathbf{d}_{\mathrm{b}} \hat{\alpha}^k, \hat{c}_{k+1} \rangle = \langle \hat{\alpha}^k, \partial_{\mathrm{i}} \hat{c}_{k+1} \rangle + \langle \hat{\alpha}^k, \partial_{\mathrm{b}} \hat{c}_{k+1} \rangle .$$

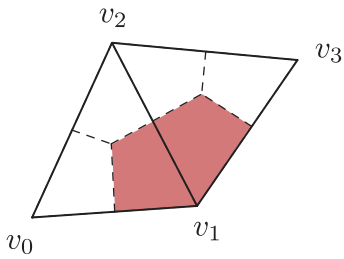


Figure 3.3: A 2-dimensional simplicial complex taken from Figure 3.3, Section 3.6, [49]. The shaded region is a Voronoi dual of the primal vertex v_1. The dual boundary, according to [49], is not the geometric boundary near the boundary of the manifold. However, in line with our construction, the boundary of the dual is the dual of the boundary.

The support volumes of a simplex and its dual cell are the same, which suggests that there is a natural identification between primal k-cochains and dual $(n-k)$-cochains.

In the exterior calculus for smooth manifolds, the Hodge star, denoted $*$, is an isomorphism between the space of k-forms and $(n-k)$-forms. Since the Hodge star operator is metric-dependent, in the discrete theory, it is defined as an equality of averages between primal and their dual forms [49, 47].

Definition 3.1.14. *The discrete Hodge star is a map* $* : \Omega_d^k(K) \to \Omega_d^{n-k}(\star_{\mathrm{i}} K)$ *defined by its value over simplices and their duals. For a* k*-simplex* σ^k*, and a discrete* k*-form* α^k*,*

$$\frac{1}{|\star_{\mathrm{i}}\, \sigma^k|}\langle *\alpha^k, \star_{\mathrm{i}}\sigma^k\rangle = \frac{1}{|\sigma^k|}\langle \alpha^k, \sigma^k\rangle\,.$$

Similarly we can define the discrete Hodge operator on the boundary, that is on an $(n-1)$-dimensional simplicial complex and its dual. It is trivial to show that for a k-form α^k the following holds: $** \alpha^k = (-1)^{k(n-k)}$.

Remark 3.1.2. *The discrete Hodge star can be represented by a matrix (see Section 3.1.4 and Section 4.1.2). According to Definition 3.1.14, this matrix is diagonal. In the case Whitney forms are used, the discrete Hodge operator is sparse but not diagonal in general [47].*

Next, we define a natural pairing, via the so-called primal-dual wedge product, between a primal k-cochain and a dual $(n-k)$-cochain. The resulting discrete form is a volume form. In order to insure anticommutativity of the primal-dual wedge product, we take the following definition.

Definition 3.1.15. *Let $\alpha^k \in \Omega_d^k(K)$ be a primal k-form and $\hat{\beta}^{n-k} \in \Omega_d^{n-k}(\star_{\mathrm{i}} K)$. We define the discrete* ***primal-dual wedge product*** $\wedge : \Omega_d^k(K) \times \Omega_d^{n-k}(\star_{\mathrm{i}} K) \to \Omega_d^n(V_k(K))$ *by*

$$\begin{aligned}\langle \alpha^k \wedge \hat{\beta}^{n-k}, V_{\sigma^k} \rangle &= \binom{n}{k} \frac{|V_{\sigma^k}|}{|\sigma^k||\star_{\mathrm{i}}\, \sigma^k|} \langle \alpha^k, \sigma^k \rangle \langle \hat{\beta}^{n-k}, \star_{\mathrm{i}} \sigma^k \rangle \\ &= \langle \alpha^k, \sigma^k \rangle \langle \hat{\beta}^{n-k}, \star_{\mathrm{i}} \sigma^k \rangle \\ &= (-1)^{k(n-k)} \langle \hat{\beta}^{n-k} \wedge \alpha^k, V_{\sigma^k} \rangle \,,\end{aligned}$$

where V_{σ^k} is the n-dimensional support volume obtained by taking the convex hull of the simplex σ^k and its dual $\star_{\mathrm{i}} \sigma^k$.

As an illustration, consider the two-dimensional simplicial complex K depicted in Figure 3.1 and its dual $\star K$ in Figure 3.2. Let $\alpha^1 \in \Omega_d^1(K)$ and $\hat{\beta}^1 \in \Omega_d^1(\star K)$. The dual cell of the primal edge $[v_k, v_i]$ is $[\hat{v}_m, \hat{v}_{m-1}]$, up to a sign depending on the chosen orientation. The primal-dual wedge product of α^1 and $\hat{\beta}^1$ on the support volume $V_{[v_k,v_i]} = V_{[\hat{v}_m,\hat{v}_{m-1}]}$, represented by the diamond shaped region generated by $[v_k, v_i]$ and $[\hat{v}_m, \hat{v}_{m-1}]$, is simply a dot product $\alpha([v_k, v_i]) \cdot \hat{\beta}^1([\hat{v}_m, \hat{v}_{m-1}])$. Now, in order to look at the primal-dual wedge product on the boundary, let $\gamma^0 \in \Omega_d^0(\partial K)$ and $\hat{\eta}^1 \in \Omega_d^1(\partial(\star K))$. For instance, $\hat{\eta}^1$ can be a restriction of $\hat{\beta}^1$ on the boundary $\partial(\star K)$. The primal-dual wedge product $\langle \gamma^0 \wedge \hat{\eta}^1, V_{v_k} \rangle = \gamma^0(v_k) \cdot \hat{\eta}^1([\hat{v}_p, \hat{v}_{p-1}])$. The volume for $V_{v_k} = V_{[\hat{v}_p,\hat{v}_{p-1}]}$ is simply the measure of the cell $[\hat{v}_p, \hat{v}_{p-1}]$.

Here we note the advantage of employing circumcentric with respect to barycentric dual since one needs to store only volume information about primal and dual cells, and not about the primal-dual convex hulls.

Definition 3.1.16. *Given two primal discrete k-forms, $\alpha^k, \beta^k \in \Omega_d^k(K)$, their discrete L^2 inner product, $\langle \alpha^k, \beta^k \rangle_d$ is given by*

$$\begin{aligned}\langle \alpha^k, \beta^k \rangle_d &= \binom{n}{k} \frac{|V_{\sigma^k}|}{|\sigma^k||\star_{\mathrm{i}}\, \sigma^k|} \langle \alpha^k, \sigma^k \rangle \langle *\beta^k, \star_{\mathrm{i}} \sigma^k \rangle \\ &= \langle \alpha^k, \sigma^k \rangle \langle *\beta^k, \star_{\mathrm{i}} \sigma^k \rangle \,.\end{aligned}$$

The proposed definition of the dual boundary operator assures the validity of the summation by parts relation that parallels the integration by parts formula for smooth differential forms.

Proposition 3.1.1. *Let K be an oriented well-centered simplicial complex. Given a primal $(k-1)$-form α^{k-1} and a dual $(n-k)$-discrete form $\hat{\beta}^{n-k}$, then*

$$\langle \mathbf{d}\alpha^{k-1} \wedge \hat{\beta}^{n-k}, K \rangle + (-1)^{k-1} \langle \alpha^{k-1} \wedge \mathbf{d}\hat{\beta}^{n-k}, K \rangle = \langle \alpha^{k-1} \wedge \hat{\beta}^{n-k}, \partial K \rangle \,,$$

where in the boundary pairing α^{k-1} is a primal $(k-1)$-form on ∂K, while $\hat{\beta}^{n-k}$ is a dual $(n-k)$-form taken on the boundary dual $\star(\partial K)$.

Proof. We have

$$\begin{aligned}\langle \mathbf{d}\alpha^{k-1} \wedge \hat{\beta}^{n-k}, K\rangle &= \sum_{\sigma^{k-1}\in K} \langle \mathbf{d}\alpha^{k-1}, \sigma^k\rangle \langle \hat{\beta}^{n-k}, \star_{\mathrm{i}}\sigma^{n-k}\rangle \\ &= \sum_{\sigma^{k-1}\in K} \langle \alpha^{k-1}, \partial\sigma^k\rangle \langle \hat{\beta}^{n-k}, \star_{\mathrm{i}}\sigma^{n-k}\rangle \\ &= \sum_{\sigma^{k-1}\in K} \sum_{\sigma^{k-1}\prec\sigma^k} \langle \alpha^{k-1}, \sigma^k\rangle \langle \hat{\beta}^{n-k}, \star_{\mathrm{i}}\sigma^{n-k}\rangle\,,\end{aligned}$$

and

$$\begin{aligned}&\langle \alpha^{k-1} \wedge \mathbf{d}\hat{\beta}^{n-k}, K\rangle \\ &= \sum_{\sigma^{k-1}} \langle \alpha^{k-1}, \sigma^{k-1}\rangle \langle \mathbf{d}\hat{\beta}^{n-k}, \star_{\mathrm{i}}\sigma^{k-1}\rangle = \sum_{\sigma^{k-1}} \langle \alpha^{k-1}, \sigma^{k-1}\rangle \langle \hat{\beta}^{n-k}, \partial(\star_{\mathrm{i}}\sigma^{k-1})\rangle \\ &= \sum_{\sigma^{k-1}} \langle \alpha^{k-1}, \sigma^{k-1}\rangle \left(\sum_{\sigma^{k-1}\prec\sigma^k} \langle \hat{\beta}^{n-k}, \star_{\mathrm{i}}(s_{\sigma^k}\sigma^k)\rangle + \langle \hat{\beta}^{n-k}, \star_{\mathrm{b}}(s_{\sigma^{k-1}}\sigma^{k-1})\rangle \right).\end{aligned}$$

Inducing the orientation of the dual such that $s_{\sigma^k} = s_{\sigma^{k-1}} = (-1)^k$ completes the proof. □

Remark 3.1.3. *Decomposing the dual form $\hat{\beta}^{n-k}$ into the internal and the boundary part as $\hat{\beta}^{n-k} = \begin{cases} \hat{\beta}_{\mathrm{i}} \in \Omega_d^{n-k}(\star_{\mathrm{i}}K) \text{ on } \star_{\mathrm{i}}K \\ \hat{\beta}_{\mathrm{b}} \in \Omega_d^{n-k}(\star_{\mathrm{b}}K) \text{ on } \partial(\star K) \end{cases}$ and decomposing the dual exterior derivative in the same manner, the summation by parts formula can be written as*

$$\langle \mathbf{d}\alpha^{k-1} \wedge \hat{\beta}_{\mathrm{i}}, K\rangle + (-1)^{k-1}\langle \alpha^{k-1} \wedge (\mathbf{d}_{\mathrm{i}}\hat{\beta}_{\mathrm{i}} + \mathbf{d}_{\mathrm{b}}\hat{\beta}_{\mathrm{b}}), K\rangle = \langle \alpha^{k-1} \wedge \hat{\beta}_{\mathrm{b}}, \partial K\rangle\,. \tag{3.1.1}$$

In the standard literature of discrete exterior calculus, the codifferential operator is adjoint to the discrete exterior derivative, with respect to the inner products of discrete forms [49]. According to Proposition 3.1.1, this is not the case since on the right a term corresponding to the primal-dual pairing on the boundary appears. As the subsequent section demonstrates, this term is precisely responsible for the inclusion of the boundary variables in the discretized Stokes-Dirac structure.

3.1.4 Matrix Representations

Discrete exterior calculus can be implemented using the formalism of linear algebra. All discrete k-forms can be stored into a vector with entries assuming the values that those forms take on the ordered set of k-simplices. The boundary operator is a linear mapping from the space of k-simplices to the space of $(k-1)$-simplices and can be represented by a sparse matrix containing only ± 1 elements, while the exterior derivative is its transpose. There is a number of different Hodge star implementations, but the so-called mass-lumped is the simplest, with the Hodge star being a diagonal matrix. The problem of standard vector representation of discrete exterior calculus will be addressed separately in the forthcoming chapter.

3.2 Dirac Structures on a Simplicial Complex

The Stokes-Dirac structure, which captures a differential symmetry of the Hamiltonian field equations, as presented in [98], is metric-independent. The essence of its construction lies in the antisymmetry of the wedge product and the Stokes theorem. In a discrete framework, the primal-primal wedge product [49] inherits a number of important properties of the cup product [73], such as bilinearity, anti-commutativity and naturality under pullback; however, it is degenerate and thus unsuitable for defining a Dirac structure. This motivates a formulation of a Dirac structure on a simplicial complex and its dual. We introduce Dirac structures with respect to the bilinear pairing between primal and duals forms on the underlying discrete manifold. We call these Dirac structures *simplicial Dirac structures*.

In the discrete setting, the smooth manifold M is replaced by an n-dimensional well-centered oriented manifold-like simplicial complex K. The flow and the effort spaces will be the spaces of complementary primal and dual forms. The elements of these two spaces are paired via the discrete primal-dual wedge product. Since the Stokes-Dirac structure $\mathcal{D}$ expresses the coupling between f_p and e_q, also f_q and e_p, via the exterior derivative, whose discrete analogue maps primal into primal and dual into dual cochains, the flow space cannot be entirely built on a primal simplicial complex and the effort space on a dual cell complex, or vice versa. Instead, the flow and the effort spaces will be mixed spaces of the primal and dual cochains. One of the two possible choices is

$$\mathcal{F}_{p,q}^{d} = \Omega_{d}^{p}(\star_{\mathrm{i}} K) \times \Omega_{d}^{q}(K) \times \Omega_{d}^{n-p}(\partial(K))$$

and

$$\mathcal{E}^d_{p,q} = \Omega^{n-p}_d(K) \times \Omega^{n-q}_d(\star_{\mathrm{i}} K) \times \Omega^{n-q}_d(\partial(\star K))\,.$$

The primal-dual wedge product ensures a bijective relation between the primal and dual forms, between the flows and efforts. A natural discrete mirror of the bilinear form (2.2.1) is a symmetric pairing on the product space $\mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q}$ defined by

$$\begin{aligned}\langle\!\langle (\underbrace{\hat{f}^1_p, f^1_q, f^1_b}_{\in \mathcal{F}^d_{p,q}}, \underbrace{e^1_p, \hat{e}^1_q, \hat{e}^1_b}_{\in \mathcal{E}^d_{p,q}}), (\hat{f}^2_p, f^2_q, f^2_b, e^2_p, \hat{e}^2_q, \hat{e}^2_b) \rangle\!\rangle_d \\ = \langle e^1_p \wedge \hat{f}^2_p + \hat{e}^1_q \wedge f^2_q + e^2_p \wedge \hat{f}^1_p + \hat{e}^2_q \wedge f^1_q, K\rangle \\ + \langle \hat{e}^1_b \wedge f^2_b + \hat{e}^2_b \wedge f^1_b, \partial K\rangle\,.\end{aligned} \tag{3.2.1}$$

A discrete analogue of the Stokes-Dirac structure is the finite-dimensional Dirac structure constructed in the following theorem.

Theorem 3.2.1 (Simplicial Dirac structure)**.** *Given linear spaces $\mathcal{F}^d_{p,q}$ and $\mathcal{E}^d_{p,q}$, and the bilinear form $\langle\!\langle , \rangle\!\rangle_d$. The linear subspace $\mathcal{D}_d \subset \mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q}$ defined by*

$$\begin{aligned}\mathcal{D}_d = \big\{ (\hat{f}_p, f_q, f_b, e_p, \hat{e}_q, \hat{e}_b) \in \mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q} \big| \\ \begin{pmatrix} \hat{f}_p \\ f_q \end{pmatrix} = \begin{pmatrix} 0 & (-1)^{pq+1}\mathbf{d}_{\mathrm{i}} \\ \mathbf{d} & 0 \end{pmatrix} \begin{pmatrix} e_p \\ \hat{e}_q \end{pmatrix} + (-1)^{pq+1} \begin{pmatrix} \mathbf{d}_{\mathrm{b}} \\ 0 \end{pmatrix} \hat{e}_b\,, \\ f_b \;=\; (-1)^p e_p|_{\partial K} \big\}\end{aligned} \tag{3.2.2}$$

is a Dirac structure with respect to the pairing $\langle\!\langle , \rangle\!\rangle_d$.

Proof. In order to show that $\mathcal{D}_d \subset \mathcal{D}_d^{\perp}$, let $(\hat{f}^1_p, f^1_q, f^1_b, e^1_p, \hat{e}^1_q, \hat{e}^1_b) \in \mathcal{D}_d$, and consider any $(\hat{f}^2_p, f^2_q, f^2_b, e^2_p, \hat{e}^2_q, \hat{e}^2_b) \in \mathcal{D}_d$. Substituting (3.2.2) into (4.2.1) yields

$$\begin{aligned}\langle (-1)^{pq+1} e^1_p \wedge \big(\mathbf{d}_{\mathrm{i}} \hat{e}^2_q + \mathbf{d}_{\mathrm{b}} \hat{e}^2_b\big) + \hat{e}^1_q \wedge \mathbf{d} e^2_p \\ + (-1)^{pq+1} e^2_p \wedge \big(\mathbf{d}_{\mathrm{i}} \hat{e}^1_q + \mathbf{d}_{\mathrm{b}} \hat{e}^1_b\big) + \hat{e}^2_q \wedge \mathbf{d} e^1_p, K\rangle \\ + (-1)^p \langle \hat{e}^1_b \wedge e^2_p + \hat{e}^2_b \wedge e^1_p, \partial K\rangle\,.\end{aligned} \tag{3.2.3}$$

By the anticommutativity of the primal-dual wedge product on K

$$\begin{aligned}\langle \hat{e}^1_q \wedge \mathbf{d} e^2_p, K\rangle &= (-1)^{q(p-1)} \langle \mathbf{d} e^2_p \wedge \hat{e}^1_q, K\rangle \\ \langle \hat{e}^2_q \wedge \mathbf{d} e^1_p, K\rangle &= (-1)^{q(p-1)} \langle \mathbf{d} e^1_p \wedge \hat{e}^2_q, K\rangle\,,\end{aligned}$$

and on the boundary ∂K

$$\begin{aligned}\langle \hat{e}_b^1 \wedge e_p^2, \partial K\rangle &= (-1)^{(p-1)(q-1)}\langle e_p^2 \wedge \hat{e}_b^1, \partial K\rangle\\ \langle \hat{e}_b^2 \wedge e_p^1, \partial K\rangle &= (-1)^{(p-1)(q-1)}\langle e_p^1 \wedge \hat{e}_b^2, \partial K\rangle\,,\end{aligned}$$

the expression (3.2.3) can be rewritten as

$$\begin{aligned}&(-1)^{q(p-1)}\langle \mathbf{d}e_p^2 \wedge \hat{e}_q^1 + (-1)^{n-p} e_p^2 \wedge \left(\mathbf{d}_{\mathrm{i}}\hat{e}_q^1 + \mathbf{d}_{\mathrm{b}}\hat{e}_b^1\right), K\rangle\\ +&(-1)^{q(p-1)}\langle \mathbf{d}e_p^1 \wedge \hat{e}_q^2 + (-1)^{n-p} e_p^1 \wedge \left(\mathbf{d}_{\mathrm{i}}\hat{e}_q^2 + \mathbf{d}_{\mathrm{b}}\hat{e}_b^2\right), K\rangle\\ &+(-1)^{p+(p-1)(q-1)}\langle \hat{e}_b^1 \wedge e_p^2 + \hat{e}_b^2 \wedge e_p^1, \partial K\rangle\,.\end{aligned}$$

According to the discrete summation by parts formula (3.1.1), the following holds

$$\begin{aligned}\langle \mathbf{d}e_p^2 \wedge \hat{e}_q^1 + (-1)^{n-p} e_p^2 \wedge \left(\mathbf{d}_{\mathrm{i}}\hat{e}_q^1 + \mathbf{d}_{\mathrm{b}}\hat{e}_b^1\right), K\rangle &= \langle e_p^2 \wedge \hat{e}_b^1, \partial K\rangle\\ \langle \mathbf{d}e_p^1 \wedge \hat{e}_q^2 + (-1)^{n-p} e_p^1 \wedge \left(\mathbf{d}_{\mathrm{i}}\hat{e}_q^2 + \mathbf{d}_{\mathrm{b}}\hat{e}_b^2\right), K\rangle &= \langle e_p^1 \wedge \hat{e}_b^2, \partial K\rangle\,.\end{aligned}$$

Hence, (3.2.3) is equal to 0, and thus $\mathcal{D}_d \subset \mathcal{D}_d^{\perp}$.

Since $\dim \mathcal{F}_{p,q}^d = \dim \mathcal{E}_{p,q}^d = \dim \mathcal{D}_d$, and $\langle\!\langle , \rangle\!\rangle_d$ is a non-degenerate form, $\mathcal{D}_d = \mathcal{D}_d^{\perp}$. □

Remark 3.2.1. *As with the continuous setting, the simplicial Dirac structure is algebraically compositional. Since the simplicial Dirac structure $\mathcal{D}_d$ is a finite-dimensional constant Dirac structure, it is integrable.*

The other possible discrete analogue of the Stokes-Dirac structure is defined on the spaces

$$\begin{aligned}\tilde{\mathcal{F}}_{p,q}^d &= \Omega_d^p(K) \times \Omega_d^q(\star_{\mathrm{i}}K) \times \Omega_d^{n-p}(\partial(\star K))\\ \tilde{\mathcal{E}}_{p,q}^d &= \Omega_d^{n-p}(\star_{\mathrm{i}}K) \times \Omega_d^{n-q}(K) \times \Omega_d^{n-q}(\partial K)\,.\end{aligned}$$

A natural discrete mirror of the bilinear form (2.2.1) in this case is a symmetric pairing on the product space $\tilde{\mathcal{F}}_{p,q}^d \times \tilde{\mathcal{E}}_{p,q}^d$ defined by

$$\begin{aligned}&\langle\!\langle (\underbrace{f_p^1, \hat{f}_q^1, \hat{f}_b^1}_{\in \tilde{\mathcal{F}}_{p,q}^d}, \underbrace{\hat{e}_p^1, e_q^1, e_b^1}_{\in \tilde{\mathcal{E}}_{p,q}^d}), (f_p^2, \hat{f}_q^2, \hat{f}_b^2, \hat{e}_p^2, e_q^2, e_b^2)\rangle\!\rangle_{\tilde{d}}\\ &\quad= \langle \hat{e}_p^1 \wedge f_p^2 + e_q^1 \wedge \hat{f}_q^2 + \hat{e}_p^2 \wedge f_p^1 + e_q^2 \wedge \hat{f}_q^1, K\rangle + \langle e_b^1 \wedge \hat{f}_b^2 + e_b^2 \wedge \hat{f}_b^1, \partial K\rangle\,.\end{aligned}$$

Theorem 3.2.2. *The linear space $\tilde{\mathcal{D}}_d$ defined by*

$$\begin{aligned}\tilde{\mathcal{D}}_d = \big\{ &(f_p, \hat{f}_q, f_b, e_p, e_q, e_b) \in \tilde{\mathcal{F}}^d_{p,q} \times \tilde{\mathcal{E}}^d_{p,q} \big| \\ &\begin{pmatrix} f_p \\ f_q \end{pmatrix} = \begin{pmatrix} 0 & (-1)^{pq+1}\mathbf{d} \\ \mathbf{d}_{\mathrm{i}} & 0 \end{pmatrix} \begin{pmatrix} \hat{e}_p \\ e_q \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbf{d}_{\mathrm{b}} \end{pmatrix} \hat{f}_b \,, \\ &e_b \;=\; (-1)^p e_q|_{\partial K} \big\}\end{aligned} \tag{3.2.4}$$

is a Dirac structure with respect to the bilinear pairing $\langle\!\langle , \rangle\!\rangle_{\tilde{d}}$.

In the following section, the simplicial Dirac structures (3.2.2) and (3.2.4) will be used as *terminus a quo* for the geometric formulation of spatially discrete port-Hamiltonian systems.

3.3 Port-Hamiltonian Systems

In the continuous theory, a distributed-parameter port-Hamiltonian system is defined with respect to the Stokes-Dirac structure (2.3.26) by imposing constitutive relations. On the other hand, in the discrete framework one can define an open Hamiltonian system with respect to the simplicial Dirac structure $\mathcal{D}_d$ or the simplicial structure $\tilde{\mathcal{D}}_d$. The choice of the structure has immediate consequence on the open dynamics since it restricts the choice of freely chosen boundary efforts or flows. Firstly, we define dynamics with respect to the structure (3.2.2) and (3.2.4). Then, in the manner of finite-dimensional port-Hamiltonian systems, we include energy dissipation by terminating some of the ports by resistive elements.

3.3.1 Port-Hamiltonian Dynamics

Let a function $\mathcal{H} : \Omega^p_d(\star_{\mathrm{i}}K) \times \Omega^q_d(K) \to \mathbb{R}$ stand for the Hamiltonian $(\hat{\alpha}_p, \alpha_q) \mapsto \mathcal{H}(\hat{\alpha}_p, \alpha_q)$, with $\hat{\alpha}_p \in \Omega^p_d(\star_{\mathrm{i}}K)$ and $\alpha_q \in \Omega^q_d(K)$. The value of the Hamiltonian after arbitrary variations of $\hat{\alpha}_p$ and α_q for $\delta\hat{\alpha}_p \in \Omega^p_d(\star_{\mathrm{i}}K)$ and $\delta\alpha_q \in \Omega^q_d(K)$, respectively, can, by Taylor expansion, be expressed as

$$\begin{aligned}\mathcal{H}(\hat{\alpha}_p + \delta\hat{\alpha}_p, \alpha_q + \delta\alpha_q) = \mathcal{H}(\hat{\alpha}_p, \alpha_q) + \langle \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p} \wedge \delta\hat{\alpha}_p + \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} \wedge \delta\alpha_q, K \rangle \\ + \text{ higher order terms in } \delta\hat{\alpha}_p, \delta\alpha_q \,.\end{aligned} \tag{3.3.1}$$

Here, it is important to emphasize that the variations $\delta\hat{\alpha}_p, \delta\alpha_q$ are not restricted to vanish on the boundary.

A time derivative of $\mathcal{H}$ along an arbitrary trajectory $t \to (\hat{\alpha}_p(t), \alpha_q(t)) \in \Omega_d^p(\star_{\mathrm{i}} K) \times \Omega_d^q(K)$, $t \in \mathbb{R}$, is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(\hat{\alpha}_p, \alpha_q) = \left\langle \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p} \wedge \frac{\partial \hat{\alpha}_p}{\partial t} + \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} \wedge \frac{\partial \alpha_q}{\partial t}, K \right\rangle . \tag{3.3.2}$$

The relation between the simplicial Dirac structure (3.2.2) and time derivatives of the variables are

$$\hat{f}_p = -\frac{\partial \hat{\alpha}_p}{\partial t}\,, \quad f_q = -\frac{\partial \alpha_q}{\partial t}\,, \tag{3.3.3}$$

while the coenergy variables are set

$$e_p = \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p}\,, \quad \hat{e}_q = \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q}\,. \tag{3.3.4}$$

This allows us to define the spatially discrete, and thus finite-dimensional, port-Hamiltonian system on a simplicial complex K (and its dual $\star K$) by

$$\begin{aligned} \begin{pmatrix} -\frac{\partial \hat{\alpha}_p}{\partial t} \\ -\frac{\partial \alpha_q}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & (-1)^r \mathbf{d}_{\mathrm{i}} \\ \mathbf{d} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p} \\ \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} \end{pmatrix} + (-1)^r \begin{pmatrix} \mathbf{d}_{\mathrm{b}} \\ 0 \end{pmatrix} \hat{e}_b\,, \\ f_b &= (-1)^p \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p}\Big|_{\partial K}\,, \end{aligned} \tag{3.3.5}$$

where $r = pq + 1$.

It immediately follows that $\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \langle \hat{e}_b \wedge f_b, \partial K \rangle$, enunciating a fundamental property of the system: the increase in the energy on the domain $|K|$ is equal to the power supplied to the system through the boundary ∂K and $\partial(\star K)$. Due to its structural properties, the system (3.3.5) can be called a spatially-discrete time-continuous boundary control system with $\hat{e}_b$ being the boundary control input and f_b being the output.

An alternative formulation of a spatially discrete port-Hamiltonian system is given in terms of the simplicial Dirac structure (3.2.4). We start with the Hamiltonian function $(\alpha_p, \hat{\alpha}_q) \mapsto \mathcal{H}(\alpha_p, \hat{\alpha}_q)$, where $\alpha_p \in \Omega_d^p(K)$ and $\hat{\alpha}_q \in \Omega_d^q(\star_{\mathrm{i}} K)$. In a similar manner as in deriving (3.3.5), we introduce the port-Hamiltonian system

$$\begin{aligned} \begin{pmatrix} -\frac{\partial \alpha_p}{\partial t} \\ -\frac{\partial \hat{\alpha}_q}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & (-1)^{pq+1} \mathbf{d} \\ \mathbf{d}_{\mathrm{i}} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_p} \\ \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_q} \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbf{d}_{\mathrm{b}} \end{pmatrix} \hat{f}_b\,, \\ e_b &= (-1)^p \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_q}|_{\partial K}\,. \end{aligned} \tag{3.3.6}$$

In contrast to (3.3.5), in the case of the formulation (3.3.6), the boundary flows $\hat{f}_b$ can be considered to be freely chosen, while the boundary efforts e_b are determined by the dynamics.

3.3.2 Modeling Dissipation

Incorporation of dissipation parallels the continuous case and for the present moment we shall consider only dissipation modeled by port termination. As an illustration, consider a mapping $\hat{R}_d : \Omega_d^q(K) \to \Omega_d^{n-q}(\star_{\mathrm{i}} K)$ that satisfies

$$\langle \hat{R}_d(f_q) \wedge f_q, K\rangle \geq 0 \quad \forall f_q \in \Omega_d^q(K)\,.$$

Furthermore, let $\hat{R}_d = R*$ with R being a positive real constant.

In case of the simplicial Dirac structure (3.2.2), introduce the relation

$$\hat{e}_q = -(-1)^{q(n-q)}\hat{R}_d(f_q) = -(-1)^{q(n-q)} R * f_q\,,$$

as well as associate to every primal $(n-p)$-cell an energy storage effort variable and to every dual p-cell a sign consistent energy flow leading to

$$\hat{f}_p = -\frac{\partial \hat{x}_p}{\partial t}\,, \quad e_p = \frac{\partial \mathcal{H}}{\partial \hat{x}}\,, \quad \hat{x} \in \Omega_d^p(\star_{\mathrm{i}} K)\,,$$

with $\mathcal{H}$ being a total stored energy.

This leads to relaxation dynamics of a diffusion process

$$\frac{\partial \hat{x}}{\partial t} = (-1)^{q-1} R\, \mathbf{d}_{\mathrm{i}} * \mathbf{d}\frac{\partial \mathcal{H}}{\partial \hat{x}} + (-1)^{pq}\mathbf{d}_{\mathrm{b}}\hat{e}_b\,,$$

with

$$\begin{aligned}
\frac{\mathrm{d}H}{\mathrm{d}t} &= \langle \frac{\partial \mathcal{H}}{\partial \hat{x}} \wedge \frac{\partial \hat{x}}{\partial t}, K\rangle \\
&= \langle \frac{\partial \mathcal{H}}{\partial \hat{x}} \wedge \left((-1)^{q-1} R\, \mathbf{d}_{\mathrm{i}} * \mathbf{d}\frac{\partial \mathcal{H}}{\partial \hat{x}} + (-1)^{pq}\mathbf{d}_{\mathrm{b}}\hat{e}_b \right), K\rangle \\
&= -R\langle \mathbf{d}\frac{\partial \mathcal{H}}{\partial \hat{x}} \wedge *\mathbf{d}\frac{\partial H}{\partial \hat{x}}, K\rangle + (-1)^p \langle \hat{e}_{\mathrm{b}} \wedge \frac{\partial \mathcal{H}}{\partial \hat{x}}, \partial K\rangle \\
&\leq \langle \hat{e}_b \wedge f_b, \partial K\rangle\,.
\end{aligned}$$

Let $\hat{f}_p = *f_p = -\frac{\partial x}{\partial t}$, $f_p, x \in \Omega_d^0(K)$, that is $p = n$ and $q = 1$. As the stored energy take $\mathcal{H} = \frac{1}{2}\langle x \wedge *x, K\rangle$. Then

$$\frac{\partial x}{\partial t} = R * \mathbf{d}_{\mathrm{i}} * \mathbf{d}x = -R\boldsymbol{\delta}\mathbf{d}x + (-1)^n \mathbf{d}_{\mathrm{b}}\hat{e}_b = -R\Delta x + (-1)^n \mathbf{d}_{\mathrm{b}}\hat{e}_b\,,$$

where Δ is the Laplace operator, $\Delta : \Omega_d^0(K) \to \Omega_d^0(K)$. One needs to be careful here with the minus sign since by the chosen convention $\Delta x = -\text{div grad}\, x$ [1]. The boundary flow is $f_b = (-1)^n x|_{\partial K}$.

Remark 3.3.1. *Consider a diffusion process on a one-dimensional simplicial complex K with a dual $\star K$ that is also a one-dimensional simplicial complex (the spatial domain is identical to the domain of the telegraph equations, confer to Figure 3.5). This means that $n = q = 1$ and $p = 0$. The operator $\hat{R}_d$ is a positive definite operator that maps the set of primal edges into the set of dual nods. The resulting dissipative port-Hamiltonian system is*

$$\frac{\partial \hat{x}}{\partial t} = \mathbf{d}_{\mathrm{i}} \hat{R}_d(\mathbf{d}x)$$

for $\hat{e}_b = 0$, which conduces to the standard compartmental model. This can be extended to structure-preserving discretization of reaction-diffusion systems as will be discussed in Chapter 6.

3.4 Physical Examples

In this section we formulate discrete analogues of distributed-parameter port-Hamiltonian systems on a three-, two-, and one-dimensional manifold.

3.4.1 Maxwell's Equations

Let K be a well-centered 3-dimensional manifold-like simplicial complex with circumcentric dual $\star K$, endowed with a discrete Riemannian metric. Mirroring the continuous case [98], we formulate the discrete Maxwell's equations in terms of discrete differential forms, and then we demonstrate that the underpinning differential/gauge structure is preserved.

The energy variables are chosen such that they live on the discrete manifolds that are dual to one another. For instance, we choose the magnetic (field) induction 2-form to be defined on the primal simplicial complex K as $\alpha_q = B \in \Omega_d^2(K)$ and the electric induction 2-form $\hat{\alpha}_p = \hat{D} \in \Omega_d^2(\star_{\mathrm{i}} K)$. This means that B and $\hat{D}$ do not reside at the same discrete locations, but rather at separate faces of staggered lattices.

Remark 3.4.1. *In the case of a spatio-temporal discretization based on the asynchronous variational integrator scheme, as proposed in [120], the electric and magnetic induction are also defined at different time locations leading to improved numerical performance (for more details refer to [120]).*

The coenergy variables are chosen coherently as implied by the choice of the energy variables such that the discrete Maxwell's equations fit the simplicial Dirac structure (3.2.2) for $n = 3$, $p = q = 2$. This entails that the magnetic field intensity $\hat{e}_q = \hat{H} \in \Omega^1_d(\star_{\mathrm{i}} K)$ and the electric intensity $e_p = E \in \Omega^1_d(K)$, as such, are related to the energy variables via

$$\begin{aligned} \hat{D} &= *\epsilon E \\ B &= *\mu \hat{H}\,, \end{aligned}$$

where ϵ and μ denote the constant electric and magnetic permittivity, respectively.

The corresponding simplicial Dirac structure is

$$\begin{aligned} \begin{pmatrix} \hat{f}_p \\ f_q \end{pmatrix} &= \begin{pmatrix} 0 & -\mathbf{d}_{\mathrm{i}} \\ \mathbf{d} & 0 \end{pmatrix} \begin{pmatrix} e_p \\ \hat{e}_q \end{pmatrix} - \begin{pmatrix} \mathbf{d}_{\mathrm{b}} \\ 0 \end{pmatrix} \hat{e}_b \\ f_b &= e_p|_{\partial K}\,. \end{aligned} \tag{3.4.1}$$

The Hamiltonian is $\mathcal{H} = \frac{1}{2}\langle E \wedge \hat{D} + \hat{H} \wedge B, K\rangle$, or expressed only in terms of the primal forms as $\mathcal{H} = \frac{1}{2}\langle E \wedge *\epsilon E + \frac{1}{\mu} * B \wedge B, K\rangle$.

Under the assumption that there is no current in the medium, the spatially discretized Maxwell's equations with respect to the simplicial Dirac structure (3.4.1) in the port-Hamiltonian form are given by

$$\begin{aligned} \begin{pmatrix} -\frac{\partial \hat{D}}{\partial t} \\ -\frac{\partial B}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & -\mathbf{d}_{\mathrm{i}} \\ \mathbf{d} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial \hat{D}} \\ \frac{\partial \mathcal{H}}{\partial B} \end{pmatrix} - \begin{pmatrix} \mathbf{d}_{\mathrm{b}} \\ 0 \end{pmatrix} \hat{e}_b \\ f_b &= \left.\frac{\partial \mathcal{H}}{\partial \hat{D}}\right|_{\partial K}\,. \end{aligned} \tag{3.4.2}$$

The readily proved energy balance is $\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \langle \hat{e}_b \wedge f_b, \partial K\rangle$. Incorporating a nonzero current density into the discrete Maxwell's equations is straightforward as in the continuous case.

3.4.2 Two-Dimensional Wave Equation

In order to demonstrate practically that we do not face a problem of interconnection of the elementary Dirac structures encountered in the mixed finite element method, as reported by [128] (see pages 183–196), we consider the simplicial Dirac structure behind the discretized two-dimensional wave equation. The normalized wave equation is given by

$$\frac{\partial^2 \phi}{\partial t^2} - \Delta \phi = 0\,,$$

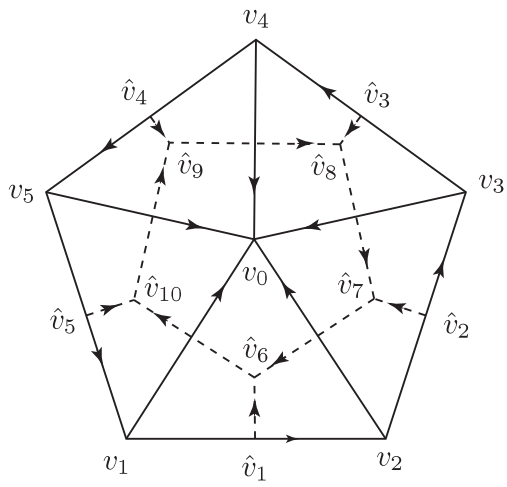


Figure 3.4: A simplicial complex K consists of five triangles arranged into a pentagon. The dual edges introduced by subdivision are shown dotted.

where ϕ is a smooth 0-form on a compact surface $M \subset \mathbb{R}^2$ with a closed boundary, and Δ is the Laplace operator. This equation, together with nonzero energy flow, can be formulated as a port-Hamiltonian system with boundary port variables [121, 39].

The energy variables of the discretized system are chosen as follows: the kinetic momentum is a dual 2-form whose time derivative is set to be $\hat{f}_p$, the elastic strain is a primal 1-form with time derivative corresponding to f_q, the coenergy variables are a primal 0-form e_p and a dual 1-form $\hat{e}_q$. Such a formulation of the discrete wave equation is consonant with the simplicial Dirac structure (3.2.2) for the case when $p = n = 2$ and $q = 1$. We shall, nevertheless, practically confirm the arguments of Theorem 4.2.1 in a simple low-dimensional model.

Consider a ring of counterclockwise oriented triangles that could be, say, obtained by a very coarse discretization of a disk. The dual of the central vertex v_0 is its Voronoi region, while the duals of the boundary vertices are the convex boundary pentagons. The orientation of the primal edges is chosen as indicated in Figure 3.4. The orientation of the dual edges is induced such that the basis of the primal and dual cells combined give the orientation of the embedding space that, in our case, has been given by the right-hand rule (for more on orientation see pages 11–22 of [49]).

It suffices to check the power conserving property of the founding Dirac

structure. We need to show that

$$\langle e_p \wedge \hat{f}_p + \hat{e}_q \wedge f_q, K\rangle + \langle \hat{e}_b \wedge f_b, \partial K\rangle = 0\,.$$

This is equivalent to the validity of the following relation

$$\langle \mathbf{d}e_p \wedge \hat{e}_q + e_p \wedge (\mathbf{d}_{\mathrm{i}}\hat{e}_q + \mathbf{d}_{\mathrm{b}}\hat{e}_b), K\rangle = \langle e_p \wedge \hat{e}_b, \partial K\rangle\,.$$

We calculate

$$\begin{aligned}
\langle \mathbf{d}e_p \wedge \hat{e}_q, K\rangle &= \sum_{\sigma^1\in K} \langle \mathbf{d}e_p, \sigma^1\rangle\langle \hat{e}_q, \star\sigma^1\rangle \\
&= \sum_{\sigma^1\in K} \langle e_p, \partial\sigma^1\rangle\langle \hat{e}_q, \star\sigma^1\rangle = \sum_{\substack{\sigma^1\in K\\ \sigma^0\prec\sigma^1}} \langle e_p, \sigma^1\rangle\langle \hat{e}_q, \star\sigma^1\rangle \\
&= (e_p(v_2) - e_p(v_1))\,\hat{e}_q([\hat{v}_1,\hat{v}_6]) + (e_p(v_3) - e_p(v_2))\,\hat{e}_q([\hat{v}_2,\hat{v}_7]) \\
&\quad + (e_p(v_4) - e_p(v_3))\,\hat{e}_q([\hat{v}_3,\hat{v}_8]) + (e_p(v_5) - e_p(v_4))\,\hat{e}_q([\hat{v}_4,\hat{v}_9]) \\
&\quad + (e_p(v_1) - e_p(v_5))\,\hat{e}_q([\hat{v}_5,\hat{v}_{10}]) + (e_p(v_0) - e_p(v_1))\,\hat{e}_q([\hat{v}_6,\hat{v}_{10}]) \\
&\quad + (e_p(v_0) - e_p(v_2))\,\hat{e}_q([\hat{v}_7,\hat{v}_6]) + (e_p(v_0) - e_p(v_3))\,\hat{e}_q([\hat{v}_8,\hat{v}_7]) \\
&\quad + (e_p(v_0) - e_p(v_4))\,\hat{e}_q([\hat{v}_9,\hat{v}_8]) + (e_p(v_0) - e_p(v_5))\,\hat{e}_q([\hat{v}_{10},\hat{v}_9])
\end{aligned}$$

and

$$\begin{aligned}
&\langle e_p \wedge (\mathbf{d}_{\mathrm{i}}\hat{e}_q + \mathbf{d}_{\mathrm{b}}\hat{e}_b), K\rangle \\
&\qquad = \sum_{\star\sigma^0\in\star K} \langle e_p, \sigma^0\rangle\langle \mathbf{d}_{\mathrm{i}}\hat{e}_q + \mathbf{d}_{\mathrm{b}}\hat{e}_b, \star\sigma^0\rangle \\
&\qquad = \sum_{\star\sigma^0\in\star K} \langle e_p, \sigma^0\rangle \left(\langle \hat{e}_q, \partial_{\mathrm{i}}(\star\sigma^0)\rangle + \langle \hat{e}_b, \partial_{\mathrm{b}}(\star\sigma^0)\rangle\right) \\
&\qquad = e_p(v_1)\Big(\hat{e}_q([\hat{v}_1,\hat{v}_6]) + \hat{e}_q([\hat{v}_6,\hat{v}_{10}]) - \hat{e}_q([\hat{v}_5,\hat{v}_{10}]) + \hat{e}_b([\hat{v}_5,\hat{v}_1])\Big) \\
&\qquad\quad + e_p(v_2)\Big(\hat{e}_q([\hat{v}_2,\hat{v}_7]) + \hat{e}_q([\hat{v}_7,\hat{v}_6]) - \hat{e}_q([\hat{v}_1,\hat{v}_6]) + \hat{e}_b([\hat{v}_1,\hat{v}_2])\Big) \\
&\qquad\quad + e_p(v_3)\Big(\hat{e}_q([\hat{v}_3,\hat{v}_8]) + \hat{e}_q([\hat{v}_8,\hat{v}_7]) - \hat{e}_q([\hat{v}_2,\hat{v}_7]) + \hat{e}_b([\hat{v}_2,\hat{v}_3])\Big) \\
&\qquad\quad + e_p(v_4)\Big(\hat{e}_q([\hat{v}_4,\hat{v}_9]) + \hat{e}_q([\hat{v}_9,\hat{v}_8]) - \hat{e}_q([\hat{v}_3,\hat{v}_8]) + \hat{e}_b([\hat{v}_3,\hat{v}_4])\Big) \\
&\qquad\quad + e_p(v_5)\Big(\hat{e}_q([\hat{v}_5,\hat{v}_{10}]) + \hat{e}_q([\hat{v}_{10},\hat{v}_9]) - \hat{e}_q([\hat{v}_4,\hat{v}_9]) + \hat{e}_b([\hat{v}_4,\hat{v}_5])\Big) \\
&\qquad\quad + e_p(v_0)\Big(- \hat{e}_q([\hat{v}_7,\hat{v}_6]) - \hat{e}_q([\hat{v}_8,\hat{v}_7]) - \hat{e}_q([\hat{v}_9,\hat{v}_8]) - \hat{e}_q([\hat{v}_{10},\hat{v}_9]) \\
&\qquad\qquad\qquad - \hat{e}_q([\hat{v}_6,\hat{v}_{10}])\Big)\,.
\end{aligned}$$

After summation of the last two relations, all terms, except those associated with the primal and dual boundary, cancel out, leading to

$$\begin{aligned}\langle \mathbf{d}e_p \wedge \hat{e}_q, K\rangle + \langle e_p \wedge (\mathbf{d}_{\mathrm{i}}\hat{e}_q + \mathbf{d}_b\hat{e}_b), K\rangle \\ = e_p(v_1)\hat{e}_b([\hat{v}_5,\hat{v}_1]) + e_p(v_2)\hat{e}_b([\hat{v}_1,\hat{v}_2]) \\ + e_p(v_3)\hat{e}_b([\hat{v}_2,\hat{v}_3]) + e_p(v_4)\hat{e}_b([\hat{v}_3,\hat{v}_4]) \\ + e_p(v_5)\hat{e}_b([\hat{v}_4,\hat{v}_5])\,.\end{aligned} \tag{3.4.3}$$

This confirms that the boundary terms genuinely live on the boundary of $|K|$.

3.4.3 Telegraph Equations

We consider an ideal lossless transmission line on a 1-dimensional simplicial complex. The energy variables are the charge density $q \in \Omega^1_d(K)$, and the flux density $\hat{\phi} \in \Omega^1_d(\star K)$, hence $p = q = 1$. The Hamiltonian representing the total energy stored in the transmission line with discrete distributed capacitance C and discrete distributed inductance L is

$$\mathcal{H} = \left\langle \frac{1}{2C} q \wedge *q + \frac{1}{2L}\hat{\phi} \wedge *\hat{\phi}, K \right\rangle ,$$

with co-energy variables: $\hat{e}_p = \frac{\partial \hat{\mathcal{H}}}{\partial q} = *\frac{q}{C} = \hat{V}$ representing voltages and $e_q = \frac{\partial \mathcal{H}}{\partial \hat{\phi}} = *\frac{\hat{\phi}}{L} = I$ currents.

Selecting $f_p = -\frac{\partial q}{\partial t}$ and $\hat{f}_q = -\frac{\partial \hat{\phi}}{\partial t}$ leads to the port-Hamiltonian formulation of the telegraph equations

$$\begin{aligned}\begin{pmatrix} -\frac{\partial q}{\partial t} \\ -\frac{\partial \hat{\phi}}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & \mathbf{d} \\ \mathbf{d}_{\mathrm{i}} & 0 \end{pmatrix} \begin{pmatrix} *\frac{q}{C} \\ *\frac{\hat{\phi}}{L} \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbf{d}_{\mathrm{b}} \end{pmatrix} \hat{f}_b \\ e_b &= -*\frac{\hat{\phi}}{L}\bigg|_{\partial K} .\end{aligned} \tag{3.4.4}$$

In the case we wanted to have the electrical current as the input, the charge and the flux density would be defined on the dual mesh and the primal mesh, respectively. Instead of the port-Hamiltonian system in the form (3.3.5), that is (3.4.4), the discretized telegraph equations would be in the form (3.3.5). The free boundary variable is always defined on the boundary of the dual cell complex.

Note that the structure (3.4.4) is in fact a Poisson structure on the state space $\Omega^1_d(K) \times \Omega^1_d(\star K)$. This will become obvious in the next chapter when we

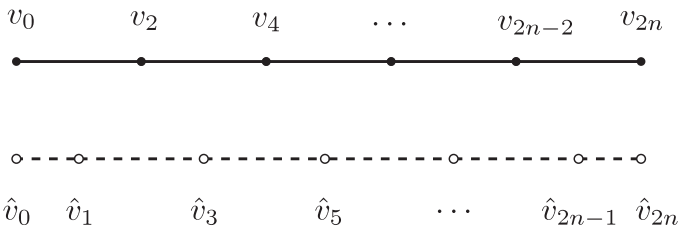


Figure 3.5: The primal 1-dimensional simplicial complex K with even nodes indices and its dual $\star K$ with odd indices, both with conventional orientation of one simplices (from the node with a lower-index to the higher-index node). By construction, the nodes $\hat{v}_0$ and $\hat{v}_{2n}$ are added to the boundary as previously explained to insure that the boundary of the dual is the dual of the boundary, i.e., $\partial(\star K) = \star(\partial K)$.

present this structure in a matrix representation. Before that, it is illustrative to demonstrate how the pairings between primal and dual forms can be rather easily calculated.

Using the notation from Figure 3.5, we have

$$\begin{aligned}
\langle \mathbf{d}e_q \wedge \hat{e}_p, K\rangle &= \sum_{\sigma^1\in K} \langle \mathbf{d}e_q, \sigma^1\rangle\langle \hat{e}_p, \star\sigma^1\rangle = \sum_{\sigma^1\in K} \langle e_q, \partial\sigma^1\rangle\langle \hat{e}_p, \star\sigma^1\rangle \\
&= (e_q(v_2) - e_q(v_0))\hat{e}_p(\hat{v}_1) + (e_q(v_4) - e_q(v_2))\hat{e}_p(\hat{v}_3) + \dots \\
&\quad + (e_q(v_{2n-2}) - e_q(v_{2n-4}))\hat{e}_p(\hat{v}_{2n-3}) \\
&\quad + (e_q(v_{2n}) - e_q(v_{2n-2}))\hat{e}_p(\hat{v}_{2n-1}) \\
&= -e_q(v_0)\hat{e}_p(\hat{v}_1) - e_q(v_2)(\hat{e}_p(\hat{v}_3) - \hat{e}_p(\hat{v}_1)) \\
&\quad - e_q(v_4)(\hat{e}_p(\hat{v}_5) - \hat{e}_p(\hat{v}_3)) \quad - \dots \\
&\quad - e_q(v_{2n-2})(\hat{e}_p(\hat{v}_{2n-1}) - \hat{e}_p(\hat{v}_{2n-3})) + e_q(v_{2n})\hat{e}_p(\hat{v}_{2n-1})
\end{aligned}$$

and

$$\begin{aligned}
\langle e_q \wedge (\mathbf{d}_{\mathrm{i}}\hat{e}_p + \mathbf{d}_{\mathrm{b}}\hat{f}_b), K\rangle &= \sum_{\star\sigma^0\in\star K} \langle e_q, \sigma^0\rangle\langle \mathbf{d}_{\mathrm{i}}\hat{e}_p + \mathbf{d}_{\mathrm{b}}\hat{f}_b, \star\sigma^0\rangle \\
&= \sum_{\star\sigma^0\in\star K} \langle e_q, \sigma^0\rangle \left(\langle \hat{e}_p, \partial_{\mathrm{i}}(\star\sigma^0)\rangle + \langle \hat{f}_b, \partial_{\mathrm{b}}(\star\sigma^0)\rangle\right) \\
&= e_q(v_0)(\hat{e}_p(\hat{v}_1) - \hat{f}_b(\hat{v}_0)) + e_q(v_2)(\hat{e}_p(\hat{v}_3) - \hat{e}_p(\hat{v}_1)) \\
&\quad + e_q(v_4)(\hat{e}_p(\hat{v}_5) - \hat{e}_p(\hat{v}_3)) + \dots \\
&\quad + e_q(v_{2n-2})(\hat{e}_p(\hat{v}_{2n-1}) - \hat{e}_p(\hat{v}_{2n-3})) \\
&\quad + e_q(v_{2n})(\hat{f}_b(\hat{v}_{2n}) - \hat{e}_p(v_{2n-1}))\,.
\end{aligned}$$

The arguments of the discrete Stokes theorem (3.1.1) are trivially verified

$$\begin{aligned}\langle \mathbf{d}e_q \wedge \hat{e}_p, K\rangle + \langle e_q \wedge (\mathbf{d}_\mathrm{i}\hat{e}_p + \mathbf{d}_\mathrm{b}\hat{f}_b), K\rangle &= \langle e_q \wedge \hat{f}_b, \partial K\rangle \\ &= -e_q(v_0)\hat{f}_b(\hat{v}_0) + e_q(v_{2n})\hat{f}_b(\hat{v}_{2n})\end{aligned}$$

showing the power-preserving property of the simplicial Dirac structure (3.4.4) which implies that for any $(\hat{e}_p, f_p, e_q, \hat{f}_q, e_b, \hat{f}_b)$ in the simplicial structure (3.4.4) the following holds

$$\langle \hat{e}_p \wedge f_p, K\rangle + \langle e_q \wedge \hat{f}_q, K\rangle + \langle e_b \wedge \hat{f}_b, \partial K\rangle = 0\,.$$

The energy balance for the transmission line thus is

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \langle e_b \wedge \hat{f}_b, \partial K\rangle = e_b(v_{2n})\hat{f}_b(\hat{v}_{2n}) - e_b(v_0)\hat{f}_b(\hat{v}_0)\,, \tag{3.4.5}$$

which demonstrates that the boundary objects genuinely live on the boundary ∂K.

3.5 Capitulation

In this chapter we have established the theoretical foundation for the formulation of Dirac structures on simplicial manifolds. Dynamical systems defined with respect to simplicial Dirac structures and their representations will be treated in the next chapter.

4
Matrix Representations

> Algebra is concerned with manipulation in time and geometry is concerned with space. These are two orthogonal aspects of the world, and they represent two different points of view in mathematics. ...
>
> One way to put the dichotomy in a more philosophical or literary framework is to say that algebra is to the geometer what you might call the 'Faustian offer'. As you know, Faust in Goethe's story was offered whatever he wanted (in his case the love of a beautiful woman), by the devil, in return for selling his soul. Algebra is the offer made by the devil to the mathematician. The devil says: "I will give you this powerful machine, it will answer any question you like. All you need to do is give me your soul: give up geometry and you will have this marvellous machine." (Nowadays you can think of it as a computer!) Of course we like to have things both ways; we would probably cheat on the devil, pretend we are selling our soul, and not give it away. Nevertheless, the danger to our soul is there, because when you pass over into algebraic calculation, essentially you stop thinking; you stop thinking geometrically, you stop thinking about the meaning.
>
> – Sir Michael Atiyah, *Mathematics in the 20th Century*

In the previous chapter I have proposed a discrete exterior geometry approach to structure-preserving discretization of distributed-parameter port-Hamiltonian systems. The spatial domain in the continuous theory represented by a finite-dimensional smooth manifold is replaced by a homological manifold-like simplicial complex and its circumcentric dual. The smooth differential forms, in discrete setting, are mirrored by cochains on the primal and dual complexes, while the discrete exterior derivative is defined to be the coboundary operator. Discrete analogues of the Stokes-Dirac structure are the so-called simplicial Dirac structures defined on spaces of primal and dual discrete differential forms. These

finite-dimensional Dirac structures offer a natural framework for the formulation of finite-dimensional port-Hamiltonian systems that emulate their infinite-dimensional counterparts. The resulting port-Hamiltonian systems are in the standard *input-output* form, unlike in [39], where the discretized models are *acausal* (given by a set of differential and algebraic equations). The explicit input-output form obtained by our scheme has the advantage from both numerical and control perspective over the implicit model presented in [39].

In this chapter I address the issue of matrix representations of simplicial Dirac structures by representing cochains by their coefficient vectors. In this manner, all linear operators from the continuous world can be represented by matrices, including the Hodge star, the coboundary and the trace operator. The simplicial Dirac structures induce a natural input-output representation of port-Hamiltonian systems. When the resulting dynamics is linear we establish bounds for the energy norms of discretization errors. I also demonstrate how these simplicial Dirac structures relate to the spatially discretized wave equation on a bounded domain and to the telegraph equations on a segment. Towards the end of the chapter, we consider the existence of structural invariants, which are crucial for the control by energy shaping.

4.1 Algebraic Aspects of Discrete Exterior Calculus

In the discrete setting, the smooth manifold M is replaced by an oriented manifold-like simplicial complex. An n-dimensional ***simplicial manifold*** K is a simplicial triangulation of an n-dimensional polytope $|K|$ with an $(n-1)$-dimensional boundary.

4.1.1 Chains and Cochains as Vectors

The discrete analogue of a smooth k-form on the manifold M is a k-cochain on the simplicial complex K. A k-chain is a formal sum of k-simplices of K such that its value on a simplex changes sign when the simplex orientation is reversed. The free Abelian group generated by a basis consisting of oriented k-simplices with real-valued coefficients is $C_k(K;\mathbb{R})$. The space $C_k(K;\mathbb{R})$ is a vector space with dimension equal to the number of k-simplices in K, which is denoted by N_k. The space of k-cochains is the vector space dual of $C_k(K;\mathbb{R})$ denoted by $C^k(K;\mathbb{R})$ or $\Omega_d^k(K)$, as a reminder that this is the ***space of discrete k-forms***.

The ***discrete exterior derivative*** or the ***coboundary operator*** $\mathbf{d}^k : \Omega_d^k(K) \to \Omega_d^{k+1}(K)$ is defined by duality to the boundary operator $\partial_{k+1} : C_{k+1}(K;\mathbb{Z}) \to$

$C_k(K;\mathbb{Z})$, with respect to the natural pairing between discrete forms and chains (cf. Definition 3.1.9). For a discrete form $\alpha \in \Omega_d^k(K)$ and a chain $c_{k+1} \in C_{k+1}(K;\mathbb{Z})$ we define $\mathbf{d}^k$ by

$$\langle \mathbf{d}^k \alpha, c_{k+1} \rangle = \langle \alpha, (\mathbf{d}^k)^{\mathrm{T}} c_{k+1} \rangle = \langle \alpha, \partial_{k+1} c_{k+1} \rangle ,$$

where the boundary operator ∂_{k+1} is the *incidence matrix* from the space of $(k+1)$-simplices to the space of k-simplices and is represented by a sparse $N_{k+1} \times N_k$ matrix containing only 0 or ± 1 elements [28]. The important property of the boundary operator is $\partial_k \circ \partial_{k+1} = 0$. The exterior derivative also satisfies $\mathbf{d}^{k+1} \circ \mathbf{d}^k = 0$, what is a discrete analogue of the vector calculus identities curl $\circ$ grad $= 0$ and div $\circ$ curl $= 0$.

Everything that has been said about the primal discrete forms carries over to the dual cochains, which can be interpreted as covectors. The space of dual k-cochains will be denoted as $\Omega_d^k(\star_{\mathrm{i}} K)$. The *covectors are labeled by a caret symbol*, e.g., $\hat{\beta} \in \Omega_d^k(\star_{\mathrm{i}} K)$.

The ***trace operator*** $\mathbf{tr}^k : \Omega_d^k(K) \to \Omega_d^k(\partial K)$ is a matrix that isolates the elements of a k-cochain vector assumed on the geometric boundary ∂K.

The ***dual exterior derivative*** $\mathbf{d}_{\mathrm{i}}^{n-k} : \Omega_d^{n-k}(\star_{\mathrm{i}} K) \to \Omega_d^{n-k+1}(\star_{\mathrm{i}} K)$ is defined by duality to the primal exterior operator $\mathbf{d}^k$ in Definition 3.1.13 assumes the matrix form

$$\mathbf{d}_{\mathrm{i}}^{n-k} = (-1)^k (\mathbf{d}^{k-1})^{\mathrm{T}} .$$

The negative sign appears as the orientation of the dual is induced by the primal orientation.

The ***dual boundary exterior derivative*** $\mathbf{d}_{\mathrm{b}}^{n-k} : \Omega_d^{n-k}(\star_{\mathrm{b}} K) \to \Omega_d^{n-k+1}(\star_{\mathrm{i}} K)$ defined in Definition 3.1.13 has the matrix representation

$$\mathbf{d}_{\mathrm{b}}^{n-k} = (-1)^{k-1} (\mathbf{tr}^{k-1})^{\mathrm{T}} .$$

For more details on geometric aspects of these operators refer to the previous chapter and for an example see Section 4.5.

4.1.2 Discrete Wedge and Hodge Operators

There exists a natural pairing, via the so-called primal-dual wedge product, between a primal k-cochain and a dual $(n-k)$-cochain. Namely, let $\alpha^k \in \Omega_d^k(K)$ and $\hat{\beta}^{n-k} \in \Omega_d^{n-k}(\star_{\mathrm{i}} K)$. We define the discrete ***primal-dual wedge product*** $\wedge : \Omega_d^k(K) \times \Omega_d^{n-k}(\star_{\mathrm{i}} K) \to \mathbb{R}$ by $\langle \alpha^k \wedge \hat{\beta}^{n-k}, V_{\sigma^k} \rangle = \langle \alpha^k, \sigma^k \rangle \langle \hat{\beta}^{n-k}, \star_{\mathrm{i}} \sigma^k \rangle =$

$(-1)^{k(n-k)}\langle \hat{\beta}^{n-k} \wedge \alpha^k, V_{\sigma^k}\rangle$, where V_{σ^k} is the n-dimensional support volume obtained by taking the convex hull of the simplex σ^k and its dual $\star_{\mathrm{i}}\sigma^k$.

The proposed definition of the dual boundary operator ensures the validity of the summation by parts relation that parallels the integration by parts formula for smooth differential forms. The matrix representation of Proposition 3.1.1 is given by the following statement.

Proposition 4.1.1 (Summation-by-parts formula)**.** *Let K be an oriented well-centered simplicial complex. Given a primal $(k-1)$-form α and an internal dual $(n-k)$-form $\hat{\beta}_{\mathrm{i}} \in \Omega_d^{n-k}(\star_{\mathrm{i}}K)$ and a dual boundary form $\hat{\beta}_{\mathrm{b}} \in \Omega_d^{n-k}(\star_{\mathrm{b}}K)$, then*

$$\langle \mathbf{d}^{k-1}\alpha \wedge \hat{\beta}_{\mathrm{i}}, K\rangle + (-1)^{k-1}\langle \alpha \wedge (\mathbf{d}_{\mathrm{i}}^{n-k}\hat{\beta}_{\mathrm{i}} + \mathbf{d}_{\mathrm{b}}^{n-k}\hat{\beta}_{\mathrm{b}}), K\rangle = \langle \mathbf{tr}^{k-1}\alpha \wedge \hat{\beta}_{\mathrm{b}}, \partial K\rangle\,.$$

Proof. For completeness, we give the simple proof. Observe that

$$\begin{aligned}
\langle \mathbf{d}^{k-1}\alpha \wedge \hat{\beta}_{\mathrm{i}}, K\rangle &= \left(\mathbf{d}^{k-1}\alpha\right)^{\mathrm{T}} \hat{\beta}_{\mathrm{i}} = \alpha^{\mathrm{t}} \left(\mathbf{d}^{k-1}\right)^{\mathrm{T}} \hat{\beta}_{\mathrm{i}} \\
&= (-1)^k \alpha^{\mathrm{T}} \mathbf{d}_{\mathrm{i}}^{n-k} \hat{\beta}_{\mathrm{i}} \\
&= (-1)^k \langle \alpha \wedge \mathbf{d}_{\mathrm{i}}^{n-k}\hat{\beta}_{\mathrm{i}}, K\rangle\,,
\end{aligned}$$

and

$$\begin{aligned}
\langle \alpha \wedge \mathbf{d}_{\mathrm{b}}^{n-k}\hat{\beta}_{\mathrm{b}}, K\rangle &= \alpha^{\mathrm{T}}\mathbf{d}_{\mathrm{b}}^{n-k}\hat{\beta}_{\mathrm{b}} = \left((\mathbf{d}_{\mathrm{b}}^{n-k})^{\mathrm{T}}\alpha\right)^{\mathrm{T}} \hat{\beta}_{\mathrm{b}} \\
&= (-1)^{k-1} \left(\mathbf{tr}^{k-1}\alpha\right)^{\mathrm{T}} \hat{\beta}_{\mathrm{b}} \\
&= (-1)^{k-1} \langle \mathbf{tr}^{k-1}\alpha \wedge \hat{\beta}_{\mathrm{b}}, \partial K\rangle\,.
\end{aligned}$$

□

The support volumes of a simplex and its dual cell are the same, which suggests that there is a natural identification between primal k-forms and dual $(n-k)$-forms. In the exterior calculus for smooth manifolds, the Hodge star, denoted $*_k$, is an isomorphism between the space of k-forms and $(n-k)$-forms. The ***discrete Hodge star*** is a map $*_k : \Omega_d^k(K) \to \Omega_d^{n-k}(\star_{\mathrm{i}}K)$ defined by its value over simplices and their duals. In case of the circumcentric duality, the Hodge star $*_k$ is a diagonal $N_k \times N_k$ matrix with the entry corresponding to a simplex σ^k being $|\star_{\mathrm{i}}\sigma^k|/|\sigma^k|$.

Another possibility for the construction of the Hodge operator is to use Whitney forms. The Whitney map is an interpolation scheme for cochains. It maps discrete forms to square integrable forms that are piecewise smooth

on each simplex. The Whitney maps are built from barycentric coordinate functions and the resulting matrix is sparse but in general *not* diagonal [15], [47].

The linear operators used in this chapter are succinctly presented in the following diagram

$$
\begin{array}{ccccccc}
\Omega_d^0(\partial K) & \xleftarrow{\mathbf{tr}^0} & \Omega_d^0(K) & \underset{*_0^{-1}}{\overset{*_0}{\rightleftarrows}} & \Omega_d^n(\star_{\mathrm{i}} K) & \xleftarrow{\mathbf{d}_{\mathrm{b}}^{n-1}} & \Omega_d^{n-1}(\star_{\mathrm{b}} K) \\
 & & \downarrow{\scriptstyle \mathbf{d}^0} & & \uparrow{\scriptstyle \mathbf{d}_{\mathrm{i}}^{n-1}} & & \\
\Omega_d^1(\partial K) & \xleftarrow{\mathbf{tr}^1} & \Omega_d^1(K) & \underset{*_1^{-1}}{\overset{*_1}{\rightleftarrows}} & \Omega_d^{n-1}(\star_{\mathrm{i}} K) & \xleftarrow{\mathbf{d}_{\mathrm{b}}^{n-2}} & \Omega_d^{n-2}(\star_{\mathrm{b}} K) \\
 & & \downarrow{\scriptstyle \mathbf{d}^1} & & \uparrow{\scriptstyle \mathbf{d}_{\mathrm{i}}^{n-2}} & & \\
\vdots & & \vdots & & \vdots & & \vdots \\
 & & \downarrow{\scriptstyle \mathbf{d}^{n-2}} & & \uparrow{\scriptstyle \mathbf{d}_{\mathrm{i}}^{1}} & & \\
\Omega_d^{n-1}(\partial K) & \xleftarrow{\mathbf{tr}^{n-1}} & \Omega_d^{n-1}(K) & \underset{*_{n-1}^{-1}}{\overset{*_{n-1}}{\rightleftarrows}} & \Omega_d^1(\star_{\mathrm{i}} K) & \xleftarrow{\mathbf{d}_{\mathrm{b}}^{0}} & \Omega_d^0(\star_{\mathrm{b}} K) \\
 & & \downarrow{\scriptstyle \mathbf{d}^{n-1}} & & \uparrow{\scriptstyle \mathbf{d}_{\mathrm{i}}^{0}} & & \\
 & & \Omega_d^n(K) & \underset{*_n^{-1}}{\overset{*_n}{\rightleftarrows}} & \Omega_d^0(\star_{\mathrm{i}} K) & &
\end{array}
\tag{4.1.1}
$$

4.2 Simplicial Dirac Structures

In this section, we develop the matrix representations of ***simplicial Dirac structures***. These structures, as we have seen in the previous chapter, are discrete analogues of the Stokes-Dirac structure and as such are defined in terms of primal and duals cochains on the underlying discrete manifold.

The role of the smooth manifold M in the discrete setting is played by an n-dimensional well-centered oriented manifold-like simplicial complex K. The flow and the effort spaces will be the spaces of complementary primal and dual forms. The elements of these two spaces are paired via the discrete primal-dual wedge product. Let

$$
\begin{aligned}
\mathcal{F}_{p,q}^d &= \Omega_d^p(\star_{\mathrm{i}} K) \times \Omega_d^q(K) \times \Omega_d^{n-p}(\partial(K)) \\
\mathcal{E}_{p,q}^d &= \Omega_d^{n-p}(K) \times \Omega_d^{n-q}(\star_{\mathrm{i}} K) \times \Omega_d^{n-q}(\partial(\star K)) \,.
\end{aligned}
$$

A natural discrete mirror of the bilinear form (2.2.1) is a symmetric pairing

on the product space $\mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q}$ defined by

$$\begin{aligned}
&\langle\!\langle (\underbrace{\hat{f}^1_p, f^1_q, f^1_b}_{\in \mathcal{F}^d_{p,q}}, \underbrace{e^1_p, \hat{e}^1_q, \hat{e}^1_b}_{\in \mathcal{E}^d_{p,q}}), (\hat{f}^2_p, f^2_q, f^2_b, e^2_p, \hat{e}^2_q, \hat{e}^2_b) \rangle\!\rangle_d \\
&\quad = \langle e^1_p \wedge \hat{f}^2_p + \hat{e}^1_q \wedge f^2_q + e^2_p \wedge \hat{f}^1_p + \hat{e}^2_q \wedge f^1_q, K \rangle \\
&\qquad + \langle \hat{e}^1_b \wedge f^2_b + \hat{e}^2_b \wedge f^1_b, \partial K \rangle \,.
\end{aligned} \tag{4.2.1}$$

A matrix analogue of the simplicial Dirac structure is the finite-dimensional Dirac structure constructed in the following theorem.

Theorem 4.2.1. *Given linear spaces $\mathcal{F}^d_{p,q}$ and $\mathcal{E}^d_{p,q}$, and the bilinear form $\langle\!\langle , \rangle\!\rangle_d$. The linear subspace $\mathcal{D}_d \subset \mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q}$ defined by*

$$\begin{aligned}
\mathcal{D}_d = \big\{ &(\hat{f}_p, f_q, f_b, e_p, \hat{e}_q, \hat{e}_b) \in \mathcal{F}^d_{p,q} \times \mathcal{E}^d_{p,q} \big| \\
&\begin{bmatrix} \hat{f}_p \\ f_q \end{bmatrix} = \begin{bmatrix} 0 & (-1)^r \mathbf{d}^{n-q}_{\mathrm{i}} \\ \mathbf{d}^{n-p} & 0 \end{bmatrix} \begin{bmatrix} e_p \\ \hat{e}_q \end{bmatrix} + (-1)^r \begin{bmatrix} \mathbf{d}^{n-q}_{\mathrm{b}} \\ 0 \end{bmatrix} \hat{e}_b \,, \\
&f_b = (-1)^p \mathbf{tr}^{n-p} e_p \big\} \,,
\end{aligned} \tag{4.2.2}$$

with $r = pq + 1$, is a Dirac structure with respect to the pairing $\langle\!\langle , \rangle\!\rangle_d$.

Proof. Note that since $\mathbf{d}^{n-q}_{\mathrm{i}} = (-1)^q (\mathbf{d}^{n-p})^{\mathrm{T}}$ and $\mathbf{d}^{n-q}_{\mathrm{b}} = (-1)^{n-p} (\mathbf{tr}^{n-p})^{\mathrm{T}}$, the operator

$$\begin{bmatrix} 0 & (-1)^r \mathbf{d}^{n-q}_{\mathrm{i}} & (-1)^r \mathbf{d}^{n-q}_{\mathrm{b}} \\ \mathbf{d}^{n-p} & 0 & 0 \\ (-1)^p \mathbf{tr}^{n-p} & 0 & \end{bmatrix}$$

is skew-symmetric, and thus (4.2.2) is a *Poisson structure* on the state space $\Omega^p_d(\star_{\mathrm{i}} K) \times \Omega^q_d(K)$. □

Remark 4.2.1. *The Dirac structure (4.2.2) is purely topological and as such does not depend on the choice of the geometric duality. Thus, the equivalent result holds in case of the barycentric duality.*

The other discrete analogue of the Stokes-Dirac structure is defined on the spaces

$$\begin{aligned}
\tilde{\mathcal{F}}^d_{p,q} &= \Omega^p_d(K) \times \Omega^q_d(\star_{\mathrm{i}} K) \times \Omega^{n-p}_d(\partial(\star K)) \\
\tilde{\mathcal{E}}^d_{p,q} &= \Omega^{n-p}_d(\star_{\mathrm{i}} K) \times \Omega^{n-q}_d(K) \times \Omega^{n-q}_d(\partial K) \,.
\end{aligned}$$

A natural discrete mirror of (2.2.1) in this case is a symmetric pairing defined by

$$\begin{aligned}&\langle\!\langle(\underbrace{f_p^1,\hat{f}_q^1,\hat{f}_b^1}_{\in\tilde{\mathcal{F}}_{p,q}^d},\underbrace{\hat{e}_p^1,e_q^1,e_b^1}_{\in\tilde{\mathcal{E}}_{p,q}^d}),(f_p^2,\hat{f}_q^2,\hat{f}_b^2,\hat{e}_p^2,e_q^2,e_b^2)\rangle\!\rangle_{\tilde{d}}\\ &=\ \langle\hat{e}_p^1\wedge f_p^2+e_q^1\wedge\hat{f}_q^2+\hat{e}_p^2\wedge f_p^1+e_q^2\wedge\hat{f}_q^1,K\rangle+\langle e_b^1\wedge\hat{f}_b^2+e_b^2\wedge\hat{f}_b^1,\partial K\rangle\,.\end{aligned}$$

Theorem 4.2.2. *The linear space $\tilde{\mathcal{D}}_d$ defined by*

$$\begin{aligned}\tilde{\mathcal{D}}_d=\big\{&(f_p,\hat{f}_q,f_b,e_p,e_q,e_b)\in\tilde{\mathcal{F}}_{p,q}^d\times\tilde{\mathcal{E}}_{p,q}^d\big|\\ &\begin{bmatrix}f_p\\ f_q\end{bmatrix}=\begin{bmatrix}0 & (-1)^{pq+1}\mathbf{d}^{n-q}\\ \mathbf{d}_{\mathrm{i}}^{n-p} & 0\end{bmatrix}\begin{bmatrix}\hat{e}_p\\ e_q\end{bmatrix}+\begin{bmatrix}0\\ \mathbf{d}_{\mathrm{b}}^{n-p}\end{bmatrix}\hat{f}_b\,,\\ &e_b\ =\ (-1)^p\mathbf{tr}^{n-q}e_q\big\}\end{aligned}\tag{4.2.3}$$

is a Dirac structure with respect to the bilinear pairing $\langle\!\langle,\rangle\!\rangle_{\tilde{d}}$.

Composition of Simplicial Dirac Structures

Consider two simplicial Dirac structures $\mathcal{D}_A$ and $\mathcal{D}_B$ defined on two simplicial manifolds K_A and K_B and their geometric duals $\star K_A$ and $\star K_B$. Furthermore, for the purpose of interconnection, let

$$\begin{aligned}\partial K_A=\Gamma_A\cup\Gamma_c\,,\quad\text{and}\quad\partial(\star K_A)=\hat{\Gamma}_A\cup\hat{\Gamma}_c\,,\\ \partial K_B=\Gamma_B\cup\Gamma_c\,,\quad\text{and}\quad\partial(\star K_B)=\hat{\Gamma}_b\cup\hat{\Gamma}_c\,,\end{aligned}$$

where $\Gamma_A,\Gamma_B,\Gamma_c$ are discrete boundaries and $\hat{\Gamma}_A,\hat{\Gamma}_B,\hat{\Gamma}_c$ are their duals. The composition $\mathcal{D}_A\circ\mathcal{D}_B$ is then defined on the primal manifold $K_A\cup K_B$ with the boundary $\Gamma_A\cup\Gamma_B$, and their duals. Since simplicial Dirac structures are finite-dimensional Dirac structures their composition is again a Dirac structure [20]. It is important to emphasize that the dual boundary $\hat{\Gamma}_c$ in general is not a geometric dual of Γ_c as Figure 4.1 illustrates it on a simple example. The implications of this in discretization are that the common dual boundary will frequently protrude over the common continuous boundary.

In the following section, the simplicial Dirac structures (4.2.2) and (4.2.3) will be used for the formulation of spatially discrete input-output port-Hamiltonian systems.

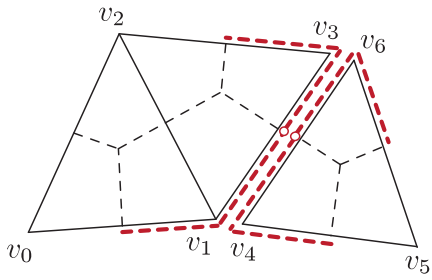


Figure 4.1: Composition of simplicial Dirac structures through the associated discrete boundary. The bold dotted line pictures the common dual boundary which protrudes out of the common primal boundary.

4.3 Input-Output Representations

Let the function $\mathcal{H} : \Omega_d^p(\star_{\mathrm{i}}K) \times \Omega_d^q(K) \to \mathbb{R}$ stand for the Hamiltonian $(\hat{\alpha}_p, \alpha_q) \mapsto \mathcal{H}(\hat{\alpha}_p, \alpha_q)$, with $\hat{\alpha}_p \in \Omega_d^p(\star_{\mathrm{i}}K)$ and $\alpha_q \in \Omega_d^q(K)$. The time derivative of $\mathcal{H}$ along an arbitrary trajectory $t \to (\hat{\alpha}_p(t), \alpha_q(t)) \in \Omega_d^p(\star_{\mathrm{i}}K) \times \Omega_d^q(K)$, $t \in \mathbb{R}$, is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(\hat{\alpha}_p, \alpha_q) = \left\langle \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p} \wedge \frac{\partial \hat{\alpha}_p}{\partial t} + \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} \wedge \frac{\partial \alpha_q}{\partial t}, K \right\rangle . \tag{4.3.1}$$

The relations between the simplicial-Dirac structure (4.2.2) and time derivatives of the variables are: $\hat{f}_p = -\frac{\partial \hat{\alpha}_p}{\partial t}$, $f_q = -\frac{\partial \alpha_q}{\partial t}$, while the efforts are: $e_p = \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p}$, $\hat{e}_q = \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q}$.

This allows us to define a time-continuous port-Hamiltonian system on a simplicial complex K (and its dual $\star K$) by

$$\begin{aligned} \begin{bmatrix} -\frac{\partial \hat{\alpha}_p}{\partial t} \\ -\frac{\partial \alpha_q}{\partial t} \end{bmatrix} &= \begin{bmatrix} 0 & (-1)^r \mathbf{d}_{\mathrm{i}}^{n-q} \\ \mathbf{d}^{n-p} & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p} \\ \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} \end{bmatrix} + (-1)^r \begin{bmatrix} \mathbf{d}_{\mathrm{b}}^{n-q} \\ 0 \end{bmatrix} \hat{e}_b \,, \\ f_b &= (-1)^p \mathbf{tr}^{n-p} \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p} \,, \end{aligned} \tag{4.3.2}$$

where $r = pq + 1$.

The system (4.3.2) is evidently in the form (2.1.6). It immediately follows that $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H} = \langle \hat{e}_b \wedge f_b, \partial K \rangle$, enunciating a fundamental property of the system: the increase in the energy on the domain $|K|$ is equal to the power supplied to the system through the boundary ∂K and $\partial(\star K)$. The boundary efforts $\hat{e}_b$ are the boundary control input and f_b are the outputs.

An alternative formulation of a spatially discrete port-Hamiltonian system is given in terms of the simplicial Dirac structure (4.2.3). We start with the Hamiltonian function $(\alpha_p, \hat{\alpha}_q) \mapsto \mathcal{H}(\alpha_p, \hat{\alpha}_q)$, where $\alpha_p \in \Omega^p_d(K)$ and $\hat{\alpha}_q \in \Omega^q_d(\star_{\mathrm{i}} K)$. In a similar manner as in deriving (4.3.2), we introduce the input-output port-Hamiltonian system

$$\begin{aligned} \begin{bmatrix} -\frac{\partial \alpha_p}{\partial t} \\ -\frac{\partial \hat{\alpha}_q}{\partial t} \end{bmatrix} &= \begin{bmatrix} 0 & (-1)^r \mathbf{d}^{n-q} \\ \mathbf{d}^{n-p}_{\mathrm{i}} & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_p} \\ \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_q} \end{bmatrix} + \begin{bmatrix} 0 \\ \mathbf{d}^{n-p}_{\mathrm{b}} \end{bmatrix} \hat{f}_b \,, \\ e_b &= (-1)^p \mathbf{tr}^{n-q} \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_q} \,. \end{aligned} \tag{4.3.3}$$

In contrast to (4.3.2), in the case of the formulation (4.3.3), the boundary flows $\hat{f}_b$ can be considered to be freely chosen, while the boundary efforts e_b are determined by the dynamics. Note that the free boundary variables are *always* defined on the boundary of the dual cell complex.

4.4 Error Analysis

In this section we consider the spatial discretization of a linear distributed-parameter port-Hamiltonian system of the form

$$\begin{aligned} -*^{\mathrm{c}}_p \frac{\partial e^{\mathrm{c}}_p}{\partial t} &= (-1)^{pq+1} \mathrm{d} e^{\mathrm{c}}_q \\ -*^{\mathrm{c}}_q \frac{\partial e^{\mathrm{c}}_q}{\partial t} &= \mathrm{d} e^{\mathrm{c}}_p \\ e^{\mathrm{c}}_q|_{\partial |K|} &= e^{\mathrm{c}}_b \\ f^{\mathrm{c}}_b &= (-1)^p e^{\mathrm{c}}_p|_{\partial |K|} \end{aligned} \tag{4.4.1}$$

on an n-dimensional polytope $|K|$. The operators $*^{\mathrm{c}}_p$ and $*^{\mathrm{c}}_q$ are the Hodge stars spawned by Riemannian metrics.

Note that all continuous (spatially undiscretized) quantities are labeled by a superscript c, for example, e^{c}_p and e^{c}_q are the continuous efforts. The approach to convergence analysis we take here is that of [48].

The discrete analogue of (4.4.1) defined with respect to the simplicial Dirac structure (4.2.2) is

$$\begin{aligned} -*_{n-p} \dot{e}_p &= (-1)^{pq+1} \left(\mathbf{d}^{n-q}_{\mathrm{i}} \hat{e}_q + \mathbf{d}^{n-q}_{\mathrm{b}} \hat{e}_b \right) \\ -*^{-1}_q \dot{\hat{e}}_q &= \mathbf{d}^{n-p} e_p \\ f_b &= (-1)^p \mathbf{tr}^{n-p} e_p \,, \end{aligned} \tag{4.4.2}$$

where $*_{n-p} \in \mathbb{R}^{N_p \times N_p}$ and $*_q^{-1} \in \mathbb{R}^{N_q \times N_q}$ are diagonal Hodge matrices with $N_p = \dim \Omega_d^{n-p}(K)$ and $N_q = \dim \Omega_d^q(K)$. A dot over a variable denotes the time derivative.

Integrate the first equation of (4.4.1) over dual p-cells and the second over primal q-faces to obtain

$$\begin{aligned} - *_{n-p} \dot{e}_p^* - \dot{\hat{r}}_p &= (-1)^{pq+1} \left(\mathbf{d}_{\mathrm{i}}^{n-q} \hat{e}_q^* + \mathbf{d}_{\mathrm{b}}^{n-q} \hat{e}_b^* \right) \\ - *_q^{-1} \dot{\hat{e}}_q^* - \dot{r}_q &= \mathbf{d}^{n-p} e_p^* \\ f_b^* &= (-1)^p \mathbf{tr}^{n-p} e_p^* , \end{aligned} \tag{4.4.3}$$

where e_p^* and $\hat{e}_q^*$ are integral forms on the primal mesh and its circumcentric dual, while $\dot{\hat{r}}_p$ and $\dot{r}_q$ are time derivatives of the residues of the Hodge operator approximations given by

$$\int_{\hat{\sigma}_k^p} *_p^{\mathrm{c}} \dot{e}_p^{\mathrm{c}} = (*_{n-p})_k \, \dot{e}_{p,k} + \left(\dot{\hat{r}}_p \right)_k \tag{4.4.4}$$

$$\int_{\sigma_l^q} *_q^{\mathrm{c}} \dot{e}_q^{\mathrm{c}} = \left(*_q^{-1} \right)_l \dot{\hat{e}}_{q,l} + (\dot{r}_q)_l \ , \tag{4.4.5}$$

with subscripts k and l acting as selectors for vector components.

Define discrete energy errors as $\delta e_p = e_p^* - e_p$ and $\delta \hat{e}_q = \hat{e}_q^* - \hat{e}_q$, and the output error as $\delta f_b = f_b^* - f_b$.

Subtracting (4.4.2) from (4.4.3) leads to

$$\begin{aligned} - *_{n-p} \delta \dot{e}_p - \dot{\hat{r}}_p &= (-1)^{pq+1} \left(\mathbf{d}_{\mathrm{i}}^{n-q} \delta \hat{e}_q + \mathbf{d}_{\mathrm{b}}^{n-q} \delta \hat{e}_b^* \right) \\ - *_q^{-1} \delta \dot{\hat{e}}_q - \dot{r}_q &= \mathbf{d}^{n-p} \delta e_p \\ \delta f_b &= (-1)^p \mathbf{tr}^{n-p} \delta e_p , \end{aligned} \tag{4.4.6}$$

since $\delta \hat{e}_b = \hat{e}_b^* - \hat{e}_b = \left(\int_{\star \sigma_b^{n-q}} e_b^{\mathrm{c}} - \langle \hat{e}_b, \star \sigma_b^{n-q} \rangle \right)_{\star \sigma_b^{n-q} \in \partial(\star K)} = 0$.

Multiplying the first equation in (4.4.6) by δe_p and the second by $\delta \hat{e}_q$ gives

$$\begin{aligned} -\langle \delta e_p, *_{n-p} \delta \dot{e}_p \rangle - \langle \delta e_p, \dot{\hat{r}}_p \rangle &= (-1)^{pq+1} \langle \delta e_p, \mathbf{d}_{\mathrm{i}}^{n-q} \delta \hat{e}_q \rangle \\ -\langle \delta \hat{e}_q, *_q^{-1} \delta \dot{\hat{e}}_q \rangle - \langle \delta \hat{e}_q, \dot{r}_q \rangle &= \langle \delta \hat{e}_q, \mathbf{d}^{n-p} \delta e_p \rangle . \end{aligned}$$

Then we have

$$\begin{aligned} &-\langle \delta e_p, *_{n-p} \delta \dot{e}_p \rangle - \langle \delta e_p, \dot{\hat{r}}_p \rangle - \langle \delta \hat{e}_q, *_q^{-1} \delta \dot{\hat{e}}_q \rangle - \langle \delta \hat{e}_q, \dot{r}_q \rangle \\ &\quad = (-1)^{pq+1} \langle \delta e_p, \mathbf{d}_{\mathrm{i}}^{n-q} \delta \hat{e}_q \rangle + \langle \delta \hat{e}_q, \mathbf{d}^{n-p} \delta e_p \rangle = 0 . \end{aligned}$$

That is

$$\langle \delta e_p, *_{n-p}\delta\dot{e}_p\rangle + \langle \delta\hat{e}_q, *_q^{-1}\delta\dot{\hat{e}}_q\rangle = -\langle \delta e_p, \dot{\hat{r}}_p\rangle - \langle \delta\hat{e}_q\dot{r}_q\rangle\,. \tag{4.4.7}$$

Integration of (4.4.7) from 0 to t_f yields

$$\begin{aligned}\frac{1}{2}\left\|(*_{n-p})^{\frac{1}{2}}\,\delta e_p(t_f)\right\|^2 + \frac{1}{2}\left\|\left(*_q^{-1}\right)^{\frac{1}{2}}\,\delta\hat{e}_q(t_f)\right\|^2 \\ = -\int_0^{t_f}\langle \delta e_p(\tau), \dot{\hat{r}}_p(\tau)\rangle + \langle \delta\hat{e}_q(\tau), \dot{r}_q(\tau)\rangle \mathrm{d}\tau \\ \leq \int_0^{t_f} \|\dot{\hat{r}}_p(\tau)\|\|\delta e_p(\tau)\| + \|\dot{r}_q(\tau)\|\|\delta\hat{e}_q(\tau)\|\mathrm{d}\tau\,.\end{aligned}$$

Let t^* be such that

$$\begin{aligned}\left\|(*_{n-p})^{\frac{1}{2}}\,\delta e_p(t^*)\right\|^2 + \left\|\left(*_q^{-1}\right)^{\frac{1}{2}}\,\delta\hat{e}_q(t^*)\right\|^2 \\ = \max_{0\leq t\leq t_f}\left(\left\|(*_{n-p})^{\frac{1}{2}}\right\|\,\|\delta e_p(t)\| + \left\|\left(*_q^{-1}\right)^{\frac{1}{2}}\right\|\,\|\delta\hat{e}_q\|\right)\,,\end{aligned}$$

then

$$\begin{aligned}&\left(\left\|(*_{n-p})^{\frac{1}{2}}\,\delta e_p(t^*)\right\| + \left\|\left(*_q^{-1}\right)^{\frac{1}{2}}\,\delta\hat{e}_q(t^*)\right\|\right)^2 \\ &\leq 2\left(\left\|(*_{n-p})^{\frac{1}{2}}\,\delta e_p(t^*)\right\|^2 + \left\|\left(*_q^{-1}\right)^{\frac{1}{2}}\,\delta\hat{e}_q(t^*)\right\|^2\right) \\ &\leq 4\int_0^{t_f}\|\dot{\hat{r}}_p(\tau)\|\|\delta e_p(\tau)\| + \|r_q(\tau)\|\,\|\delta\hat{e}_q(\tau)\|\,\mathrm{d}\tau \\ &\leq 4\int_0^{t_f}\left(\left\|(*_{n-p})^{\frac{1}{2}}\,\delta e_p(t)\right\| + \left\|\left(*_q^{-1}\right)^{\frac{1}{2}}\,\delta\hat{e}_q(t)\right\|\right) \\ &\qquad\cdot\left(\left\|(*_{n-p})^{\frac{1}{2}}\,\dot{\hat{r}}_p(\tau)\right\| + \left\|\left(*_q^{-1}\right)^{\frac{1}{2}}\,\dot{r}_q(\tau)\right\|\right)\mathrm{d}\tau\,.\end{aligned}$$

It follows that

$$\begin{aligned}&\left\|(*_{n-p})^{\frac{1}{2}}\,\delta e_p(t^*)\right\| + \left\|\left(*_q^{-1}\right)^{\frac{1}{2}}\,\delta\hat{e}_q(t^*)\right\| \\ &\leq 4\int_0^{t_f}\left\|(*_{n-p})^{-\frac{1}{2}}\,\dot{\hat{r}}_p(\tau)\right\| + \left\|\left(*_q^{-1}\right)^{-\frac{1}{2}}\,\dot{r}_q(\tau)\right\|\mathrm{d}\tau\,.\end{aligned}$$

Thus

$$\begin{aligned}\|\delta e_p(t^*)\| + \|\delta\hat{e}_q(t^*)\| \leq 4\left(\|\,(*_{n-p})^{-\frac{1}{2}}\,\|_\infty + \|\,\left(*_q^{-1}\right)^{-\frac{1}{2}}\,\|_\infty\right) \\ \cdot\int_0^{t_f}\|\,(*_{n-p})^{-\frac{1}{2}}\,\dot{\hat{r}}_p(\tau)\| + \|\,\left(*_q^{-1}\right)^{-\frac{1}{2}}\,\dot{r}_q(\tau)\|\mathrm{d}\tau\,.\end{aligned}$$

Estimation of the residues $\hat{r}_p$ and r_q can be conducted by employing Bramble-Hilbert techniques in the case of a weak formulation, or using a Taylor's expansion of the efforts under the standard smoothness assumptions [47]. For the results on the estimates of the Hodge star in one, two and three dimension the reader is invited to consult [47] and references therein.

4.5 Revisiting Physical Examples

In this section we consider the discrete wave equation on a 2-dimensional simplicial complex and the telegraph equations on a segment.

4.5.1 Two-Dimensional Wave Equation

Consider the wave equation $\mu \frac{\partial^2 u^c}{\partial t^2} = -E\Delta u^c$, with $u^c(t,z) \in \mathbb{R}$, $z = (z_1, z_2) \in M$, where μ is the mass density, E is the Young's modulus, Δ is the two-dimensional Laplace operator, and M is a compact surface with a closed boundary. Throughout, the superscript c designates the continuous quantities.

The energy variables are the 2-dimensional kinetic momentum p^c, and the 1-form elastic strain ϵ^c. The coenergy variables are the 0-form velocity v^c and the 1-form stress σ^c. The energy density of the vibrating membrane is $\mathcal{H}(p,\epsilon) = \frac{1}{2}(\epsilon^c \wedge \sigma^c + p^c \wedge v^c)$, where the coenergy and energy variables are related by the constitutive relations $\sigma^c = E * \epsilon^c$ and $v^c = 1/\mu * p^c$. The Hodge operator here corresponds to the standard Euclidian metric on M. The full details of the port-Hamiltonian formulation of the vibrating membrane is given in [39].

Let us now consider the simplicial Dirac structure underpinning the discretized two-dimensional wave equation. The energy variables of the discretized system are chosen as follows: the kinetic momentum is a dual 2-form whose time derivative is set to be $\hat{f}_p$, the elastic strain is a primal 1-form with time derivative corresponding to f_q, the coenergy variables are a primal 0-form e_p and a dual 1-form $\hat{e}_q$. Such a formulation of the discrete wave equation is consonant with the simplicial Dirac structure (4.2.2) for the case when $p = n = 2$ and $q = 1$, and is given by

$$\begin{aligned} \begin{bmatrix} \hat{f}_p \\ f_q \end{bmatrix} &= \begin{bmatrix} 0 & -\mathbf{d}^1_{\mathrm{i}} \\ \mathbf{d}^0 & 0 \end{bmatrix} \begin{bmatrix} e_p \\ \hat{e}_q \end{bmatrix} - \begin{bmatrix} \mathbf{d}^1_{\mathrm{b}} \\ 0 \end{bmatrix} \hat{e}_b \,, \\ f_b &= \mathbf{tr}^0 e_p \,. \end{aligned}$$

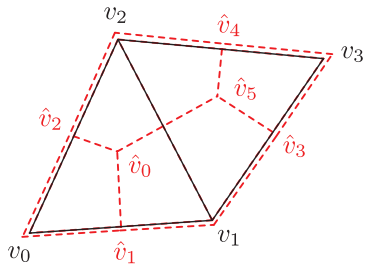


Figure 4.2: A simplicial complex K consists of two triangles. The dual edges introduced by subdivision are shown dotted.

The boundary control variable is the 1-form stress $\hat{e}_b$, while the output is the boundary velocity. The Hamiltonian of the discrete model is

$$\mathcal{H} = \frac{1}{2}\left\langle \epsilon \wedge E *_1 \epsilon + \hat{p} \wedge \frac{1}{\mu} *_0^{-1} \hat{p}, K \right\rangle .$$

The coenergy variables are the dual 1-form $\hat{\sigma} = \frac{\partial \mathcal{H}}{\partial \epsilon} = E *_1 \epsilon$ and the primal 0-form $v = \frac{\partial \mathcal{H}}{\partial \hat{p}} = *_0^{-1}\hat{p}$.

The resulting port-Hamiltonian system is

$$\begin{aligned}
\begin{bmatrix} \frac{\partial \hat{p}}{\partial t} \\ \frac{\partial \epsilon}{\partial t} \end{bmatrix} &= \begin{bmatrix} 0 & \mathbf{d}^1_{\mathrm{i}} \\ -\mathbf{d}^0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\mu} *_0^{-1} & 0 \\ 0 & E *_1 \end{bmatrix} \begin{bmatrix} \hat{p} \\ \epsilon \end{bmatrix} + \begin{bmatrix} \mathbf{d}^1_{\mathrm{b}} \\ 0 \end{bmatrix} \hat{e}_b \\
f_b &= \frac{1}{\mu} \mathbf{tr}^0 *_0^{-1} \hat{p} \,,
\end{aligned}$$

where the operators $\mathbf{d}^0$, $\mathbf{d}^1_i$, $\mathbf{tr}^0 = (\mathbf{d}^1_{\mathrm{b}})^{\mathrm{T}}$, $*_1$, and $*_0^{-1}$ conform to the diagram (4.1.1) when $n = 2$.

Example 4.5.1. *Consider a simplicial complex pictorially given by Fig. 4.2. The primal and dual 2-faces have counterclockwise orientations. The matrix representation of the incidence operator ∂_1, from the primal edges to the primal vertices, is*

	$[v_0, v_1]$	$[v_1, v_2]$	$[v_2, v_0]$	$[v_1, v_3]$	$[v_3, v_2]$
v_0	-1	0	0	0	0
v_1	1	-1	0	-1	0
v_2	0	1	-1	0	1
v_3	0	0	1	1	-1

while the discrete exterior derivative from the vertices to the edges is the transpose of the incidence operator, i.e., $\mathbf{d}^0 = \partial_1^{\mathrm{T}}$. *The dual exterior derivative is* $\mathbf{d}_{\mathrm{i}}^1 = -\left(\mathbf{d}^0\right)^{\mathrm{T}}$, *while the matrix representation of the* $\mathbf{d}_{\mathrm{b}}^1$ *operator is*

	$[\hat{v}_2, \hat{v}_1]$	$[\hat{v}_1, \hat{v}_3]$	$[\hat{v}_3, \hat{v}_4]$	$[\hat{v}_4, \hat{v}_2]$
$\star_{\mathrm{i}} v_0$	1	0	0	0
$\star_{\mathrm{i}} v_1$	0	1	0	0
$\star_{\mathrm{i}} v_2$	0	0	0	1
$\star_{\mathrm{i}} v_3$	0	0	1	0

The trace operator is $\mathbf{tr}^0 = (\mathbf{d}_{\mathrm{b}}^1)^{\mathrm{T}}$.

It is trivial to show

$$\begin{aligned} &\langle \mathbf{d}^0 e_p \wedge \hat{e}_q, K\rangle + \langle e_p \wedge (\mathbf{d}_{\mathrm{i}}^1 \hat{e}_q + \mathbf{d}_{\mathrm{b}}^1 \hat{e}_b), K\rangle \\ &= \hat{e}_b[\hat{v}_2, \hat{v}_1] f_b(v_0) + \hat{e}_b[\hat{v}_1, \hat{v}_3] f_b(v_1) \\ &\quad + \hat{e}_b[\hat{v}_3, \hat{v}_4] f_b(v_3) + \hat{e}_b[\hat{v}_4, \hat{v}_2] f_b(v_2)\,, \end{aligned} \tag{4.5.1}$$

what confirms that the boundary terms genuinely live on the boundary of $|K|$.

If the geometric duality is circumcentric, the diagonal Hodge operators are

$$\begin{aligned} *_0 &= \operatorname{diag}\left(|\star_{\mathrm{i}} v_0|, |\star_{\mathrm{i}} v_1|, |\star_{\mathrm{i}} v_2|, |\star_{\mathrm{i}} v_3|\right) \\ *_1 &= \operatorname{diag}\left(\frac{|[\hat{v}_1, \hat{v}_0]|}{|[v_0, v_1]|}, \frac{|[\hat{v}_0, \hat{v}_5]|}{|[v_1, v_2]|}, \frac{|[\hat{v}_2, \hat{v}_0]|}{|[v_2, v_0]|}, \frac{|[\hat{v}_3, \hat{v}_5]|}{|[v_1, v_3]|}, \frac{|[\hat{v}_4, \hat{v}_5]|}{|[v_3, v_2]|}\right). \end{aligned}$$

4.5.2 Telegraph Equations

We consider an ideal lossless transmission line on a 1-dimensional simplicial complex (see Figure 3.5). The energy variables are the charge density $q \in \Omega_d^1(K)$, and the flux density $\hat{\phi} \in \Omega_d^1(\star K)$, hence $p = q = 1$. The Hamiltonian representing the total energy stored in the transmission line with distributed capacitance C and distributed inductance $\hat{L}$ is

$$\mathcal{H} = \left\langle \frac{1}{2C} q \wedge *_1 q + \frac{1}{2\hat{L}} \hat{\phi} \wedge *_0^{-1} \hat{\phi}, K \right\rangle, \tag{4.5.2}$$

where $*_0$ and $*_1$ are the discrete diagonal Hodge operators that relate the appropriate cochains according to the following schematic diagram

$$\begin{array}{ccccc} \Omega_d^0(\partial K) & \xleftarrow{\mathbf{tr}^0} & \Omega_d^0(K) & \xrightarrow{\mathbf{d}^0} & \Omega_d^1(K) \\ \downarrow *_{\mathrm{b}} & & \downarrow *_0 & & \downarrow *_1 \\ \Omega_d^0(\partial(\star K)) & \xrightarrow{\mathbf{d}_{\mathrm{b}}^0} & \Omega_d^1(\star_{\mathrm{i}} K) & \xleftarrow{\mathbf{d}_{\mathrm{i}}^0} & \Omega_d^0(\star_{\mathrm{i}} K)\,, \end{array}$$

where $\star_{\mathrm{b}}$ is the identity.

The co-energy variables are: $\hat{e}_p = \frac{\partial \hat{\mathcal{H}}}{\partial q} = *\frac{q}{C} = \hat{V}$ representing voltages, and $e_q = \frac{\partial \mathcal{H}}{\partial \hat{\phi}} = *\frac{\hat{\phi}}{\hat{L}} = I$ currents. Selecting $f_p = -\frac{\partial q}{\partial t}$ and $\hat{f}_q = -\frac{\partial \hat{\phi}}{\partial t}$ leads to the port-Hamiltonian formulation of the telegraph equations

$$\begin{aligned} \begin{bmatrix} -\frac{\partial q}{\partial t} \\ -\frac{\partial \phi}{\partial t} \end{bmatrix} &= \begin{bmatrix} 0 & \mathbf{d}^0 \\ \mathbf{d}_{\mathrm{i}}^0 & 0 \end{bmatrix} \begin{bmatrix} *_1 \frac{q}{C} \\ *_0^{-1} \frac{\hat{\phi}}{\hat{L}} \end{bmatrix} + \begin{bmatrix} 0 \\ \mathbf{d}_{\mathrm{b}}^0 \end{bmatrix} \hat{f}_b \\ e_b &= -\mathbf{tr}^0 *_0^{-1} \frac{\hat{\phi}}{\hat{L}}, \end{aligned} \tag{4.5.3}$$

where $\hat{f}_b$ are the input voltages and e_b are the output currents.

In the case we want to have the electrical currents as the inputs, the charge and the flux densities would be defined on the dual mesh and the primal mesh, respectively. Instead of the port-Hamiltonian system in the form (4.5.3), the discretized telegraph equations would be in the form (4.3.2). The charge density is defined on the dual cell complex as $\hat{q} \in \Omega_d^1(\star_{\mathrm{i}} K)$ and the discrete flux density is $\phi \in \Omega_d^1(K)$. The finite-dimensional port-Hamiltonian system is of the form

$$\begin{aligned} \begin{bmatrix} -\frac{\partial \hat{q}}{\partial t} \\ -\frac{\partial \phi}{\partial t} \end{bmatrix} &= \begin{bmatrix} 0 & \mathbf{d}_{\mathrm{i}}^0 \\ \mathbf{d}^0 & 0 \end{bmatrix} \begin{bmatrix} *_0^{-1} \frac{\hat{q}}{\hat{C}} \\ *_1 \frac{\phi}{L} \end{bmatrix} + \begin{bmatrix} \mathbf{d}_{\mathrm{b}}^0 \\ 0 \end{bmatrix} \hat{e}_b \\ f_b &= -\mathbf{tr}^0 *_0^{-1} \frac{\hat{q}}{\hat{C}}, \end{aligned} \tag{4.5.4}$$

where $\hat{e}_b$ are the input currents and f_b are the output voltages.

The exterior derivative $\mathbf{d}^0 : \Omega_d^0(K) \to \Omega_d^1(K)$ is the transpose of the incidence matrix of the primal mesh. The discrete derivative $\mathbf{d}_{\mathrm{i}}^0 : \Omega_d^0(\star_{\mathrm{i}} K) \to \Omega_d^1(\star_{\mathrm{i}} K)$ in the matrix notation is the incidence matrix of the primal mesh. Thus, we have

$$-(\mathbf{d}_{\mathrm{i}}^0)^{\mathrm{T}} = \mathbf{d}^0 = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ & & & \ddots & & \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix}, \tag{4.5.5}$$

$$\mathbf{tr}^0 = (\mathbf{d}_{\mathrm{b}}^0)^{\mathrm{T}} = \begin{bmatrix} -1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix}. \tag{4.5.6}$$

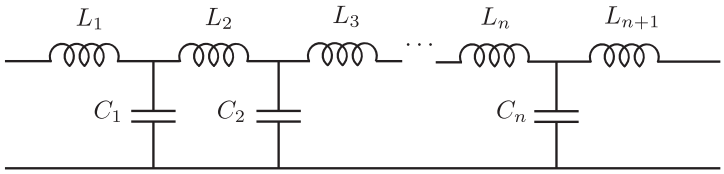


Figure 4.3: The finite-dimensional approximation of the lossless transmission line when the inputs are voltages and the outputs are currents. The inductances $L_1, \ldots, L_{n+1}$ are the values that the discrete distributed inductance $\hat{L}$ takes on the simplices $[\hat{v}_0, \hat{v}_1], \ldots, [\hat{v}_{2n-1}, \hat{v}_{2n}]$; the capacitances $C_1, \ldots C_n$ are the values C takes on $[v_0, v_2], \ldots, [v_{2n-2}, v_{2n}]$.

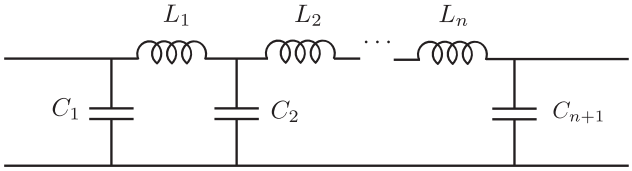


Figure 4.4: The finite-dimensional approximation of the lossless transmission line when the inputs are currents and the outputs are voltages. The inductances are: $L_1 = \int_{[v_0,v_2]} L^c = L([v_0, v_2])$, $L_2 = \int_{[v_2,v_4]} L^c = L([v_2, v_4])$, $\ldots$, $L_n = \int_{[v_{2n-2},v_{2n}]} L^c = L([v_{2n-2}, v_{2n}])$; the values of capacitors are: $C_1 = \int_{[\hat{v}_0,\hat{v}_1]} C^c = \hat{C}([\hat{v}_0, \hat{v}_1])$, $C_2 = \int_{[\hat{v}_1,\hat{v}_3]} C^c = \hat{C}([\hat{v}_1, \hat{v}_3])$, $C_3 = \int_{[\hat{v}_3,\hat{v}_5]} C^c = \hat{C}([\hat{v}_3, \hat{v}_5])$, $\ldots$, $C_{n+1} = \int_{[\hat{v}_{2n-1},\hat{v}_{2n}]} C^c = \hat{C}([\hat{v}_{2n-1}, \hat{v}_{2n}])$.

Remark 4.5.1. *The discrete analogue of the Stokes-Dirac structure obtained in [39] is a finite-dimensional Dirac structure, but not a Poisson structure (4.2.2) or (4.2.3). The implication of this on the physical realization is that, in contrast to our results, the transmission line in the finite-dimensional case is not only composed of inductors and capacitors but also of transformers.*

The physical realizations of the port-Hamiltonian systems (4.5.3) and (4.5.4) are given on Fig. 4.3 and Fig. 4.4, respectively. Stabilization of either of those systems is easily achieved by terminating boundary ports with resistive elements.

Error Analysis for the Telegraph Equations

Expressing the flows of (4.5.3) in terms of efforts and choosing $L = C = 1$ for convenience, the matrix formulation of (4.5.3) is

$$\begin{aligned} -(*_1)^{-1}\,\dot{\hat{e}}_p &= \mathbf{d}^0 e_q \\ -*_0\,\dot{e}_q &= -\mathbf{d}_{\mathrm{i}}^0 \hat{e}_p - \mathbf{d}_{\mathrm{b}}^0 \hat{f}_b \\ e_b &= -\mathbf{tr}^0 e_q\,, \end{aligned} \tag{4.5.7}$$

where $(*_1)^{-1} = \mathrm{diag}(h_1, h_3, \ldots, h_{2n-1}) \in \mathbb{R}^{n\times n}$ and $*_0 = \mathrm{diag}\left(\hat{h}_0, \hat{h}_2, \ldots, \hat{h}_{2n}\right)$ $\in \mathbb{R}^{(n+1)\times(n+1)}$, with $h_1 = |[v_0, v_2]|$, $h_3 = |[v_2, v_4]|$, $\ldots$, $h_{2n-1} = |[v_{2n-2}, v_{2n}]|$ and $\hat{h}_0 = |[\hat{v}_0, \hat{v}_1]|$, $\hat{h}_2 = |[\hat{v}_1, \hat{v}_3]|$, $\ldots$, $\hat{h}_{2n} = |[\hat{v}_{2n-1}, \hat{v}_{2n}]|$.

The time derivatives of the r_p components defined in (4.4.4) are

$$(\dot{r}_p)_l = h_{2l-1}\dot{e}_p(\hat{v}_{2l-1}) - \int_{[v_{2l-1}, v_{2l}]} *\dot{e}_p^{\mathrm{c}} = h_{2l-1}\dot{e}_p(\hat{v}_{2l-1}) - \int_{v_{2l-1}}^{v_{2l}} \dot{e}_p^{\mathrm{c}}(z)\mathrm{d}z\,.$$

The Taylor's expansion of $\dot{e}_p^{\mathrm{c}}$ around $\hat{v}_{2l-1}$ is

$$\dot{e}_p^{\mathrm{c}}(z) = \dot{e}_p^{\mathrm{c}}(\hat{v}_{2l-1}) + \frac{\partial \dot{e}_p^{\mathrm{c}}}{\partial z}(\hat{v}_{2l-1})(z - \hat{v}_{2l-1}) + \frac{\partial^2 \dot{e}_p^{\mathrm{c}}}{\partial z^2}(\hat{v}_{2l-1})\frac{(z - \hat{v}_{2l-1})^2}{2} + O(z^3)\,.$$

Thus

$$\int_{v_{2l-2}}^{v_{2l}} \dot{e}_p^{\mathrm{c}}(z)\mathrm{d}z = \dot{e}_p^{\mathrm{c}}(\hat{v}_{2l-1})h_{2l-1} + \frac{1}{3}\frac{\partial^2 \dot{e}_p^{\mathrm{c}}}{\partial z^2}(\hat{v}_{2l-1})\left(\frac{\hat{h}_{2l}}{2}\right)^3 + O(h_{2l}^4)\,,$$

and

$$(\dot{r}_p)_l = \frac{1}{3}\frac{\partial^2 \dot{e}_p^{\mathrm{c}}}{\partial z^2}(\hat{v}_{2l-1})\left(\frac{h_{2l}}{2}\right)^3 + O(h_{2l}^4)\,.$$

Likewise $\big($cf. (4.4.5)$\big)$,

$$\left(\dot{\hat{r}}_q\right)_{k+1} = \hat{h}_{2k}\dot{e}_q(v_{2k}) - \int_{[\hat{v}_{2k-1}, \hat{v}_{2k+1}]} *\dot{e}_q^{\mathrm{c}} = \hat{h}_{2k}\dot{e}_q(v_{2k}) - \int_{\hat{v}_{2k-1}}^{\hat{v}_{2k+1}} \dot{e}_q^{\mathrm{c}}(z)\mathrm{d}z\,,$$

where $k = 0, 1, \ldots, n$ and $\hat{v}_{-1} = \hat{v}_0$. In the similar fashion, we obtain

$$\begin{aligned} \left(\dot{\hat{r}}_q\right)_{k+1} &= \frac{1}{3}\frac{\partial^2 \dot{e}_q^{\mathrm{c}}}{\partial z^2}(v_{2k})\left(\frac{\hat{h}_{2k}}{2}\right)^3 + O(\hat{h}_{2k}^4) \ \text{ for } \ k = 1, \ldots, n-1 \\ \left(\dot{\hat{r}}_q\right)_1 &= \frac{1}{2}\frac{\partial \dot{e}_q^{\mathrm{c}}}{\partial z}(v_0)\hat{h}_0^2 + O(\hat{h}_0^3) \\ \left(\dot{\hat{r}}_q\right)_{n+1} &= -\frac{1}{2}\frac{\partial \dot{e}_q^{\mathrm{c}}}{\partial z}(v_{2n})\hat{h}_{2n}^2 + O(\hat{h}_{2n}^3)\,. \end{aligned}$$

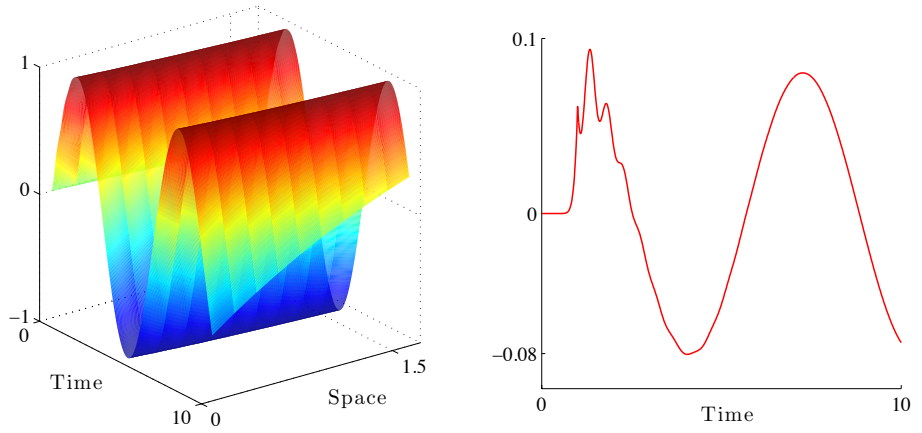


Figure 4.5: On the left, the voltage distribution e_p for $n = 10$, and on the right, the voltage error at the point $z = \mathrm{e} - 1$, that is $e_b(v_{20})(t) - \sin(t-1)$ for $t \geq 0$.

It follows that there exist $K_1, K_2 \in \mathbb{R}$ such that

$$\|\delta\hat{e}_p(t^*)\| + \|\delta e_q(t^*)\| \leq hK_2 \int_0^{t_f} \|\mathbf{tr}^0 \frac{\partial \dot{e}_q^{\mathrm{c}}}{\partial z}(\tau)\| \mathrm{d}\tau + h^2 K_1 \int_0^{t_f} \left(\|\frac{\partial^2 \dot{e}_p^{\mathrm{c}}}{\partial z^2}(\tau)\| + \|\frac{\partial^2 \dot{e}_q^{\mathrm{c}}}{\partial z^2}(\tau)\| \right) \mathrm{d}\tau + O(h^3) \tag{4.5.8}$$

where $\mathbf{tr}^0$ is a trace operator, $\mathbf{tr}^0 = \left(\mathbf{d}_{\mathrm{b}}^0\right)^{\mathrm{T}}$, and h is the measure of mesh quality $h = \min\{h_1, h_3, \ldots, h_{2n-1}, \hat{h}_0, \hat{h}_2, \ldots, \hat{h}_{2n}\}$.

Numerical example. To evince how exactly the discrete model relates to the continuous one, we take the example from Section 5 in [39].

The spatial domain of the transmission system is the line segment $M = [0, \mathrm{e} - 1]$. The distributed capacitance and the distributive inductance are $z \mapsto C^{\mathrm{c}}(z) = \frac{1}{1+z}$ and $z \mapsto L^{\mathrm{c}}(z) = \frac{1}{1+z}$, $z \in M$. On the left-hand side a causal input voltage $t \mapsto u(t)$ is assigned, and at the other end the transmission line is terminated by a load of unit resistance, meaning $*q(t, \mathrm{e} - 1) = *\phi(t, \mathrm{e} - 1)$. Initial conditions are assumed to be zero, i.e. $q^{\mathrm{c}}(0, z) = 0$ and $\phi^{\mathrm{c}}(0, z) = 0$ for $z \in Z$. The exact solution for the voltage distribution is $(t, z) \mapsto e_p^{\mathrm{c}}(t, z) = u(t - \ln(z + 1))$, for $t \geq 0$.

Using equidistant division of M and diagonal Hodge operators, the results of numerical simulation when the input $e_p^{\mathrm{c}}(0, t) = u(t) = \sin t$, $t \geq 0$, are

given in Figure 4.5. The time integration technique is Runge-Kutta 4 and the integration step is 0.01.

All numerical experiments indicate that the discrepancy between the exact value of the voltage and the value obtained by numerical simulation is the greatest at the spatial point $z = \mathrm{e} - 1$. Thence, in the left-hand side of Figure 4.5 we show this error as a function of time. In all computational experiments, this error, similar to the results in [39], exhibits an oscillatory behavior with the amplitude not exceeding the maximum displayed in the first period.

Repeating simulation experiments for uniform grids of different densities indicates that the accuracy of the proposed method is $1/n$, what comes as no surprise since we worked with diagonal Hodge operators, which are of first-order accuracy as shown in (4.5.8) for the system (4.5.3).

4.6 Conservation Laws

Let us consider the existence of conservation laws and structural invariants for the port-Hamiltonian systems on simplicial complexes.

4.6.1 Finite-Dimensional Invariants

The following proposition gives the conditions for the existence of conservation laws in the discrete setting.

Proposition 4.6.1. *Consider the port-Hamiltonian system (4.3.2). Let* $(\hat{\alpha}_p, \alpha_q) \mapsto C(\hat{\alpha}_p, \alpha_q)$ *be a real-valued function. Then,* C *is a conservation law for the port-Hamiltonian system (4.3.2) satisfying*

$$\frac{\mathrm{d}C}{\mathrm{d}t} = \left(f_b^C\right)^{\mathrm{T}} \hat{e}_b \tag{4.6.1}$$

with $f_b^C = -(-1)^{q(p+1)} \mathbf{tr}^{n-p} \frac{\partial C}{\partial \hat{\alpha}_p}$, *if and only if*

$$\frac{\partial C}{\partial \hat{\alpha}_p} \in \ker \mathbf{d}^{n-p} \tag{4.6.2}$$

$$\frac{\partial \hat{C}}{\partial \alpha_q} \in \ker \mathbf{d}_{\mathrm{i}}^{n-q}\,. \tag{4.6.3}$$

Proof. Differentiating C along the flow of the system (4.3.2), we have

$$\begin{aligned}\frac{\mathrm{d}C}{\mathrm{d}t} &= \left\langle \frac{\partial C}{\partial \hat{\alpha}_p} \wedge \frac{\partial \hat{\alpha}_p}{\partial t} + \frac{\partial \hat{C}}{\partial \alpha_q} \wedge \frac{\partial \alpha_q}{\partial t}, K \right\rangle \\ &= (-1)^{pq} \frac{\partial^{\mathrm{T}} C}{\partial \hat{\alpha}_p} \left(\mathbf{d}_{\mathrm{i}}^{n-q} \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} + \mathbf{d}_{\mathrm{b}}^{n-q} \hat{e}_b \right) - (-1)^{q(n-q)} \left(\mathbf{d}^{n-q} \frac{\partial \mathcal{H}}{\alpha_q} \right)^{\mathrm{T}} \frac{\partial \hat{C}}{\partial \alpha_q} \\ &= (-1)^{q(p+1)} \left(\mathbf{d}^{n-p} \frac{\partial C}{\partial \hat{\alpha}_p} \right)^{\mathrm{T}} \frac{\partial \hat{\mathcal{H}}}{\partial \alpha_q} - (-1)^{q(p+1)} \left(\mathbf{tr}^{n-p} \frac{\partial C}{\partial \hat{\alpha}_p} \right)^{\mathrm{T}} \hat{e}_b \\ &\quad + (-1)^{pq} \left(\mathbf{d}_{\mathrm{i}}^{n-q} \frac{\partial \hat{C}}{\partial \alpha_q} \right)^{\mathrm{T}} \frac{\partial \mathcal{H}}{\partial \hat{\alpha}_p},\end{aligned}$$

because $\mathbf{d}_{\mathrm{i}}^{n-q} = (-1)^q (\mathbf{d}^{n-p})^{\mathrm{T}}$ and $\mathbf{d}_{\mathrm{b}}^{n-q} = (-1)^{n-p} (\mathbf{tr}^{n-p})^{\mathrm{T}}$. Furthermore, regardless of $\mathcal{H}$, the result (4.6.1) follows iff (4.6.2) and (4.6.3) hold. □

Remark 4.6.1. *If either $\hat{e}_b = 0$ or $f_b^C = 0$, the quantity C satisfying (4.6.2) and (4.6.3) is a conserved quantity—a Casimir function.*

4.6.2 One-Dimensional Domain

An interesting case for which it is possible explicitly to solve (4.6.2) is when $p = n$. The matrix $\mathbf{d}^0$ is nothing but the transpose of the incidence matrix ∂_1, from the set of edges to the set of vertices, of a connected graph. It is a well-known property of the incidence matrix ∂_1 that $\ker \partial_1^{\mathrm{T}} = \operatorname{span} \mathbf{1}$, where $\mathbf{1}$ stands for the vector with all elements equal 1. A direct consequence of this is that $\frac{\partial C}{\partial \hat{\alpha}_p} = \mathbf{1}$ up to a multiplicative constant.

In the one-dimensional case the null space of $\mathbf{d}_{\mathrm{i}}^0$ is trivial, cf. (4.5.5), what allows us to explicitly express the conservation law.

Corollary 4.6.2. *Consider the port-Hamiltonian system (4.3.2), with $p = q = n = 1$, on the one-dimensional simplicial manifold given on Figure 3.5. The quantity $C_p = \mathbf{1}^{\mathrm{T}} \hat{\alpha}_p = \hat{\alpha}_p([\hat{v}_0, \hat{v}_1]) + \sum_{k=1}^{n-1} \hat{\alpha}_p([\hat{v}_{2k-1}, \hat{v}_{2k+1}]) + \hat{\alpha}_p([\hat{v}_{2n-1}, \hat{v}_{2n}])$ satisfies the balance law*

$$\frac{\mathrm{d}C_p}{\mathrm{d}t} = \hat{e}_b(\hat{v}_0) - \hat{e}_b(\hat{v}_{2n}). \tag{4.6.4}$$

In case of the telegraph equations on the segment $M = [0, 1]$, the total charge $C_q^c = \int_0^1 q^c(t, z)\mathrm{d}z$ as well as the total magnetic flux $C_\phi^c = \int_0^1 \phi^c(t, z)\mathrm{d}z$ are both conservation laws. In the discrete setting, the *only* conservation law for the system (4.5.4) is the total charge $C_q = \mathbf{1}^{\mathrm{T}} \hat{q}$ whose derivative along

the admissible trajectories is $\frac{\mathrm{d}C_q}{\mathrm{d}t} = \hat{e}_b(\hat{v}_0) - \hat{e}_b(\hat{v}_{2n})$. Similarly, the total flux $C_\phi = \mathbf{1}^{\mathrm{T}}\hat{\phi}$ in the system (4.5.3) satisfies the balance law $\frac{\mathrm{d}C_\phi}{\mathrm{d}t} = \hat{f}_b(\hat{v}_0) - \hat{f}_b(\hat{v}_{2n})$, where $\hat{f}_b(\hat{v}_0)$ and $\hat{f}_b(\hat{v}_{2n})$ are input currents. These result differ from those presented in [63], where both the total flux and total charge are conserved.

4.7 Energy-Casimir Method

Consider the interconnection of (4.3.2) with the (possibly nonlinear) integrator

$$\frac{\mathrm{d}\zeta}{\mathrm{d}t} = \mathbf{g}_c\, u_c \tag{4.7.1}$$

$$y_c = \mathbf{g}_c^{\mathrm{T}} \frac{\partial H_c}{\partial \zeta}\,, \tag{4.7.2}$$

where $\zeta \in \mathbb{R}^m$, $\mathbf{g}_c \in \mathbb{R}^{m\times N_b}$ with $N_b = \dim \Omega_d^{n-q}(\partial(\star K))$, input u_c, output y_c, and $\zeta \mapsto H_c(\zeta)$ the controller's Hamiltonian. The interconnection is power-preserving with $u_c = f_b$ and $e_b = -y_c$. The composition is the port-Hamiltonian system in the form

$$\begin{bmatrix} \frac{\partial \hat{\alpha}_p}{\partial t} \\ \frac{\partial \alpha_q}{\partial t} \\ \frac{\mathrm{d}\zeta}{\mathrm{d}t} \end{bmatrix} = \begin{bmatrix} 0 & (-1)^{r-1}\mathbf{d}_{\mathrm{i}}^{n-q} & (-1)^r \mathbf{d}_{\mathrm{b}}^{n-q}\mathbf{g}_c^{\mathrm{T}} \\ \mathbf{d}^{n-p} & 0 & 0 \\ (-1)^p \mathbf{g}_c\, \mathbf{tr}^{n-p} & 0 & \end{bmatrix} \begin{bmatrix} \frac{\partial H_{\mathrm{cl}}}{\partial \hat{\alpha}_p} \\ \frac{\partial \hat{H}_{\mathrm{cl}}}{\partial \alpha_q} \\ \frac{\partial H_{\mathrm{cl}}}{\partial \zeta} \end{bmatrix}, \tag{4.7.3}$$

with $(\hat{\alpha}_p, \alpha_q, \zeta) \mapsto H_{\mathrm{cl}}(\hat{\alpha}_p, \alpha_q, \zeta)$ is the closed-loop Hamiltonian $H_{\mathrm{cl}}(\hat{\alpha}_p, \alpha_q, \zeta) = \mathcal{H}(\hat{\alpha}_p, \alpha_q) + H_c(\zeta)$.

The energy shaping for the system (4.7.3) is achieved by restricting the behavior of (4.7.3) to a certain subspace [96]. To this end, we look at the Casimir functions of the closed-loop system.

Proposition 4.7.1. *The real-valued function $(\hat{\alpha}_p, \alpha_q, \zeta) \mapsto C(\hat{\alpha}_p, \alpha_q, \zeta)$ is a Casimir function of the closed system (4.7.3) iff*

$$\begin{aligned} \frac{\partial C}{\partial \hat{\alpha}_p} &\in \ker \mathbf{d}^{n-p} \cap \ker\left(\mathbf{g}_c\, \mathbf{tr}^{n-p}\right) \\ \begin{bmatrix} \frac{\partial \hat{C}}{\partial \alpha_q} \\ \frac{\partial C}{\partial \zeta} \end{bmatrix} &\in \ker \begin{bmatrix} \mathbf{d}_{\mathrm{i}}^{n-q} & (-1)^{n-q}\mathbf{d}_{\mathrm{b}}^{n-q}\mathbf{g}_c^{\mathrm{T}} \end{bmatrix}. \end{aligned} \tag{4.7.4}$$

Proof. Solving $\frac{\mathrm{d}}{\mathrm{d}t}C(\hat{\alpha}_p, \alpha_q, \zeta) = 0$ irrespective of H_{cl} directly leads to (4.7.4). □

Remark 4.7.1. *Since the structural matrix of the port-Hamiltonian system (4.3.2) is* not *of full rank in case when* $\mathbf{g}_c$ *is identity, not all Casimirs of (4.7.3) are of the form* $C(\hat{\alpha}_q, \alpha_q, \zeta) = S_i(\hat{\alpha}_p, \alpha_q) - \zeta_i$, $i = 1, \ldots, m$.

Remark 4.7.2. *In case when* $p = q = m = n = 1$ *and* $\mathbf{g}_c = [1, 1]$ *the* only *Casimir for the system (4.7.3) is* $\mathbf{1}^{\mathrm{T}}\alpha_q + \zeta$.

4.8 Final Remarks

By preserving the Hamiltonian structure, the methodology of this chapter utilizes the analysis and control synthesis for the discretized systems.

An important avenue for future research is to make a connection between continuous and discretized systems in the presence of a port-Hamiltonian controller. Here, gauging the input-output errors is of great significance for robustness.

5
Symmetry Reduction

> In beauty, that of favor, is more than that of color; and that of decent and gracious motion, more than that of favor. That is the best part of beauty, which a picture cannot express; no, nor the first sight of the life. There is no excellent beauty, that hath not some strangeness in the proportion.
>
> – Sir Francis Bacon, *Of Beauty*

The port-Hamiltonian formalism, as we have seen, transcends the lumped-parameter scenario and has been successfully applied to study of a number of distributed-parameter systems stemming from mechanics, electromagnetism and chemistry [98, 64, 107]. The centerpiece of the efforts concerning infinite-dimensional case is the Stokes-Dirac structure. The Hamiltonian equations associated to this Dirac structure allow for non-zero energy exchange through the boundary.

Although the differential operator in the Stokes-Dirac structure, in the presence of nonzero boundary conditions, is not skew-symmetric, it is possible to associate a Poisson structure to the Stokes-Dirac structure [98]. In the absence of algebraic constraints imposed by boundary conditions, the Stokes-Dirac structure specializes to a Poisson structure [29], and as such it can be derived through symmetry reduction from a canonical Dirac structure on the phase space [127]. How to conduct this reduction for the Poisson structure associated to the Stokes-Dirac structure on a manifold with boundary is the central theme of this chapter.

This chapter very closely follows [127]. The reduction scheme we are dealing with is the one from [127], the only difference being in that we consider slightly augmented spaces in order to account for the behaviors associated with the boundary. The perspective as well as the notation in Section 5.1 are taken verbatim from [127], but now for the generalized Dirac structures that

allow for the formulation of open Hamiltonian systems. The proposed Poisson reduction is firstly applied in the reduction of a generalized canonical Dirac structure to the Poisson structure associated with the Stokes-Dirac structure. In the context of dynamics, the canonical port-Hamiltonian systems are those defined as in [102, 103], now only in the context of differential forms, while the reduced port-Hamiltonian systems are exactly those presented in [98]. In the final section I demonstrate how this reduction applies to the Poisson reduction of the port-Hamiltonian systems on simplicial manifolds [110, 109].

5.1 Dirac Structures and Reduction

Dirac structures. Let $\mathcal{Q}$ be a manifold and define a pairing on $T\mathcal{Q} \oplus T^*\mathcal{Q}$ given by

$$\langle\langle (v,\alpha),(w,\beta)\rangle\rangle = \frac{1}{2}(\alpha(w)+\beta(v)).$$

For a subspace $\mathcal{D}$ of $T\mathcal{Q} \oplus T^*\mathcal{Q}$, we define the orthogonal complement $\mathcal{D}^\perp$ as the space of all (v,α) such that $\langle\langle (v,\alpha),(w,\beta)\rangle\rangle = 0$ for all (w,β). A ***Dirac structure*** is then a subbundle $\mathcal{D}$ of $T\mathcal{Q} \oplus T^*\mathcal{Q}$ which satisfies $\mathcal{D} = \mathcal{D}^\perp$.

The canonical Dirac structure. Let $\mathcal{Q}$ be equipped with a symplectic form ω and note that ω induces a map $\flat : T\mathcal{Q} \to T^*\mathcal{Q}$ given by $\flat(v) = \mathbf{i}_v\omega$ for $v \in T\mathcal{Q}$. Since ω is symplectic, $\flat$ can be inverted and we denote the inverse map by $\sharp : T^*\mathcal{Q} \to T\mathcal{Q}$, referred to as the ***Poisson structure*** induced by ω. It can easily checked that the graph of $\flat$ (or equivalently of $\sharp$), given by

$$\begin{aligned}\mathcal{D}_{T^*\mathcal{Q}} &:= \{(v,\flat(v)) : v \in T\mathcal{Q}\} \\ &= \{(\sharp(\alpha),\alpha) : \alpha \in T^*\mathcal{Q}\} \end{aligned} \tag{5.1.1}$$

is a Dirac structure. In the literature [127], [135] a Dirac structure given by (5.1.1) is called a ***canonical Dirac structure***.

The notion of Dirac structures just entertained is suitable for the formulation of *closed* Hamiltonian systems, however, our aim is a treatment of *open* Hamiltonian systems in such a way that some of the external variables remain free port variables. For this reason we recall the notion of the augmented (generalized) Dirac structure.

The augmented Dirac structures. In addition to the configuration manifold $\mathcal{Q}$, let $\mathcal{F}$ be a linear vector space of *external flows*, with dual the space $\mathcal{F}^*$ of *external efforts*. We deal with Dirac structures on the product space $\mathcal{Q} \times \mathcal{F}$.

The pairing on $(T\mathcal{Q} \times \mathcal{F}) \oplus (T^*\mathcal{Q} \times \mathcal{F})$ is given by

$$\begin{aligned} &\left\langle\!\left\langle \Big((v,f),(\alpha,e)\Big), \Big((w,\tilde{f}),(\beta,\tilde{e})\Big) \right\rangle\!\right\rangle \\ &\quad = \Big(\alpha(w) + e(\tilde{f}) + \beta(v) + \tilde{e}(f)\Big)\,. \end{aligned} \tag{5.1.2}$$

An ***augmented Dirac structure*** $\mathcal{D}$ is a subbundle of $(T\mathcal{Q} \times \mathcal{F}) \oplus (T^*\mathcal{Q} \times \mathcal{F})$ which is maximally isotropic under (5.1.2).

A canonical Dirac structure on $T\mathcal{Q} \oplus T^*\mathcal{Q}$ is considered to be a symplectic structure (5.1.1). However, in this thesis we shall deal with slightly different canonical Dirac structures. To that end, let the map $\sharp : T^*\mathcal{Q} \times \mathcal{F}^* \to T\mathcal{Q} \times \mathcal{F}$ induce a ***Poisson structure*** on $T\mathcal{Q} \times \mathcal{F}$. The graph of $\sharp$ given by

$$\mathcal{D}_{T^*\mathcal{Q}\times\mathcal{F}^*} := \{(\sharp(\alpha,e),(\alpha,e)) : \alpha \in T^*\mathcal{Q}\,, e \in \mathcal{F}^*\} \tag{5.1.3}$$

is a Dirac structure. If the mapping $\sharp$ is symplectic on $T\mathcal{Q}$, that is if $\sharp(\alpha,0) = 0$ implies $\alpha = 0$, the Dirac structure (5.1.3) is the ***generalized canonical Dirac structure***.

Example 5.1.1. *Let $(v,f) \in T\mathcal{Q} \times \mathcal{F}$, and $(\alpha,e) \in T^*\mathcal{Q} \times \mathcal{F}^*$. If $J = -J^*$ and $\ker J = 0$, then*

$$\begin{pmatrix} v \\ f \end{pmatrix} = \begin{pmatrix} J & -g \\ g^* & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ e \end{pmatrix}$$

is a generalized canonical Dirac structure. Note that, if $\mathcal{F} = \emptyset$, we are dealing with a symplectic structure.

Reduction of Dirac structures. There is a number of techniques for symmetry reduction of Dirac structures [13, 135]. The reduction considered in this chapter is the Poisson reduction from [127]. For that purpose, let $\mathfrak{G}$ be a Lie group which acts on $\mathcal{Q}$ from the right and assume that the quotient space $\mathcal{Q}/\mathfrak{G}$ is again a manifold. Denote the action of $\mathfrak{g} \in \mathfrak{G}$ on $q \in \mathcal{Q}$ by $q \cdot \mathfrak{g}$ and the induced actions of $\mathfrak{g} \in \mathfrak{G}$ on $T\mathcal{Q} \times \mathcal{F}$ and $T^*\mathcal{Q} \times \mathcal{F}^*$ by $(v,f) \cdot \mathfrak{g}$ and $(\alpha,e) \cdot \mathfrak{g}$, for $v \in T\mathcal{Q}$, $f \in \mathcal{F}$, $\alpha \in T^*\mathcal{Q}$, and $e \in \mathcal{F}^*$. The action on the $T^*\mathcal{Q} \times \mathcal{F}^*$ is defined by $\langle (\alpha,e) \cdot \mathfrak{g}, (v,f) \rangle = \langle (\alpha,e), (v,f) \cdot \mathfrak{g}^{-1} \rangle$. In what follows, we will focus mostly on the reduced cotangent bundle $(T^*\mathcal{Q} \times \mathcal{F}^*)/\mathfrak{G}$. Furthermore, we will deal with the reduced space denoted by $T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*$.

Consider now the canonical Dirac structure on $T^*\mathcal{Q} \times \mathcal{F}^*$. Let $\sharp : T^*\mathcal{Q} \times \mathcal{F}^* \to T\mathcal{Q} \times \mathcal{F}$ be the map (5.1.3) used in the definition of $\mathcal{D}_{T^*\mathcal{Q}\times\mathcal{F}^*}$. The reduced Dirac structure $\mathcal{D}_{T^*\mathcal{Q}/\mathfrak{G}\times\mathcal{F}^*}$ on $T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*$ can now be described as the graph of a reduced map $[\sharp] : T^*(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*) \to T(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*)$ defined as follows.

Let $\pi_G : T^*\mathcal{Q} \times \mathcal{F}^* \to T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*$ be the quotient map and consider an element (ρ, π, ρ_b) in $T^*\mathcal{Q} \times \mathcal{F}^*$. The tangent map of $\pi_{\mathfrak{G}}$ at (ρ, π, ρ_b) is denoted by $T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}} : T_{(\rho,\pi,\rho_b)}(T^*\mathcal{Q} \times \mathcal{F}^*) \to T_{(\rho,\pi,\rho_b)}(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*)$, and its dual by $T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}} : T^*_{\pi_{\mathfrak{G}}(\rho,\pi,\rho_b)}(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*) \to T^*_{\pi_{\mathfrak{G}}(\rho,\pi,\rho_b)}(T^*\mathcal{Q} \times \mathcal{F}^*)$. The reduced map $[\sharp]$ now fits into the following extended commutative diagram

$$\begin{array}{ccc} T^*_{(\rho,\pi,\rho_b)}(T^*\mathcal{Q} \times \mathcal{F}^*) & \xrightarrow{\quad\sharp\quad} & T_{(\rho,\pi,\rho_b)}(T^*\mathcal{Q} \times \mathcal{F}^*) \\ \uparrow{\scriptstyle T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}} & & \downarrow{\scriptstyle T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}} \\ T^*_{\pi_{\mathfrak{G}}(\rho,\pi,\rho_b)}(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*) & \xrightarrow[[\sharp]]{} & T_{\pi_{\mathfrak{G}}(\rho,\pi,\rho_b)}(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*) \end{array} \tag{5.1.4}$$

5.2 Properties of the Stokes-Dirac Structure

As usual, throughout the chapter, let M be an oriented n-dimensional smooth manifold with a smooth $(n-1)$-dimensional boundary ∂M endowed with the induced orientation, representing the space of spatial variables. By $\Omega^k(M)$, $k = 0, 1, \ldots, n$, denote the space of exterior k-forms on M, and by $\Omega^k(\partial M)$, $k = 0, 1, \ldots, n-1$, the space of k-forms on ∂M. A natural non-degenerative pairing between $\rho \in \Omega^k(M)$ and $\sigma \in \Omega^{n-k}(M)$ is given by $\langle \sigma | \rho \rangle = \int_M \sigma \wedge \rho$. Likewise, the pairing on the boundary ∂M between $\rho \in \Omega^k(\partial M)$ and $\sigma \in \Omega^{n-k-1}(\partial M)$ is given by $\langle \sigma | \rho \rangle = \int_{\partial M} \sigma \wedge \rho$.

The Stokes-Dirac structure. For any pair p, q of positive integers satisfying $p + q = n + 1$, define the flow and effort linear spaces by

$$\begin{aligned} \mathcal{F}_{p,q} &= \Omega^p(M) \times \Omega^q(M) \times \Omega^{n-p}(\partial M) \\ \mathcal{E}_{p,q} &= \Omega^{n-p}(M) \times \Omega^{n-q}(M) \times \Omega^{n-q}(\partial M)\,. \end{aligned}$$

Given linear spaces $\mathcal{F}_{p,q}$ and $\mathcal{E}_{p,q}$, and the natural bilinear form $\langle\!\langle , \rangle\!\rangle$, we recall that the bundle $\mathcal{D} \subset \mathcal{F}_{p,q} \times \mathcal{E}_{p,q}$

$$\begin{aligned} \mathcal{D} = \big\{ (f_p, f_q, f_b, e_p, e_q, e_b) \in \mathcal{F}_{p,q} \times \mathcal{E}_{p,q} \big| \\ \begin{pmatrix} f_p \\ f_q \end{pmatrix} = \begin{pmatrix} 0 & (-1)^{pq+1}\mathrm{d} \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix}, \\ \begin{pmatrix} f_b \\ e_b \end{pmatrix} = \begin{pmatrix} \mathrm{tr} & 0 \\ 0 & -(-1)^{n-q}\mathrm{tr} \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix} \big\}, \end{aligned} \tag{5.2.1}$$

is the Stokes-Dirac structure.

Poisson brackets on the Stokes-Dirac structure. Although Dirac structures generalize the notion of Poisson structures, to any Stokes-Dirac structure we can associate a Poisson structure. Here we just sketch the essence and refer the reader to [98].

We define the space of admissible efforts as

$$\mathcal{E}_{\text{adm}} := \{e \in \mathcal{E}_{p,q} | \exists f \in \mathcal{F}_{p,q} \text{ such that } (f,e) \in \mathcal{D}\}.$$

On $\mathcal{E}_{\text{adm}}$ define the bilinear form $[e_1, e_2] = \langle e_1 | f_2 \rangle \in \mathbb{R}$, where $f_2 \in \mathcal{F}_{p,q}$ is such that $(f_2, e_2) \in \mathcal{D}$. This bilinear form is well-defined, since for any $f_2' \in \mathcal{F}$ such that $(f_2', e_2) \in \mathcal{D}$ we obtain by linearity $(f_2 - f_2', 0) \in \mathcal{D}$, and hence $0 = \langle\langle (f_1, e_1), (f_2 - f_2', 0) \rangle\rangle = \langle e_1 | f_2 \rangle - \langle e_1 | f_2' \rangle$. Furthermore, $[,]$ is skew-symmetric since for any (f_1, e_1), $(f_2, e_2) \in \mathcal{D}$ we have $0 = \langle\langle (f_1, e_1), (f_2, e_2) \rangle\rangle = \langle e_1 | f_2 \rangle + \langle e_2 | f_1' \rangle$.

The set of admissible mappings is now defined to be

$$\begin{aligned}\mathcal{K}_{\text{adm}} = \{k : \mathcal{F}_{p,q} \to \mathbb{R} | \forall a \in \mathcal{F}_{p,q},\ \exists e(k,a) \in \mathcal{E}_{\text{adm}} \text{ such that} \\ \forall a \in \mathcal{F}_{p,q},\ k(a + \partial a) = k(a) + \langle e(k,a) | \partial a \rangle + O(\partial a)\}.\end{aligned}$$

Notice that $e(k,a)$, if it exists, is uniquely defined modulo the following linear space $\mathcal{E}_0 = \{e \in \mathcal{E}_{p,q} | \langle e | f \rangle = 0 \text{ for all } f \in \mathcal{F}_{p,q}\}$, which is a subspace of $\mathcal{E}_{p,q}$. The quantity $e(k,a)$ is the derivative of k at a, and we denote it by $\delta k(a)$. On $\mathcal{K}_{\text{adm}}$ we define the bracket $\{k_1, k_2\}_{\mathcal{D}}(a) = [\delta k_1(a), \delta k_2(a)]$, for any $k_1, k_2 \in \mathcal{K}_{\text{adm}}$. This bracket is clearly independent from the choice of the representations $\delta k_1(a), \delta k_2(a)$. By skew-symmetry of $[,]$ it immediately follows that $\{,\}$ is skew-symmetric.

For the Stokes-Dirac structure the set of admissible mappings $\mathcal{K}_{\text{adm}}$ consists of those functions $k : \Omega^p(M) \times \Omega^q(M) \times \Omega^{n-p}(\partial M) \to \mathbb{R}$ whose derivatives $\delta k(z) = (\delta_p k(z), \delta_q k(z), \delta_b k(z)) \in \Omega^{n-p}(M) \times \Omega^{n-q}(M) \times \Omega^{n-q}(\partial M)$ satisfy

$$\delta_b k(z) = -(-1)^{n-q} \text{tr}(\delta_q k(z)).$$

The Poisson bracket on $\mathcal{K}_{\text{adm}}$ is given as

$$\begin{aligned}\{k^1, k^2\}_{\mathcal{D}} = \int_M ((\delta_p k^1) \wedge (-1)^r \text{d}((\delta_q k^2) + (\delta_q k^1) \wedge \text{d}(\delta_p k^2)) \\ - \int_{\partial M} ((-1)^{n-q} (\delta_q k^1) \wedge (\delta_p k^2)).\end{aligned}$$

Using Stokes' theorem, it follows that the bracket is skew-symmetric and that it satisfies the Jacobi identity: $\{\{k^1, k^2\}_{\mathcal{D}}, k^3\}_{\mathcal{D}} + \{\{k^2, k^3\}_{\mathcal{D}}, k^1\}_{\mathcal{D}} + \{\{k^3, k^1\}_{\mathcal{D}}, k^2\}_{\mathcal{D}} = 0$ for all $k^i \in \mathcal{K}_{\text{adm}}$.

In this chapter we will exclusively be dealing with Poisson and associated Poisson structures.

5.3 Reduction of the Stokes-Dirac Structure

The configuration manifold is a vector space $\mathcal{Q} := \Omega^k(M)$ with the tangent bundle $T\mathcal{Q} = \mathcal{Q} \times \mathcal{Q}$ and the cotangent bundle $T^*\mathcal{Q} = \mathcal{Q} \times \mathcal{Q}^*$, where $\mathcal{Q}^* = \Omega^{n-k}(M)$. The space of the boundary flows $\mathcal{F}$ will be an admissible subset of $\Omega^{n-k-1}(\partial M)$, while the space of the boundary efforts is $\mathcal{E} := \mathcal{F}^* = \Omega^k(\partial M)$.

The tangent bundle $T(T^*\mathcal{Q} \times \mathcal{F}^*)$ is isomorphic to $(\mathcal{Q} \times \mathcal{Q}^* \times \mathcal{F}^*) \times (\mathcal{Q} \times \mathcal{Q}^* \times \mathcal{F}^*)$, with a typical element denoted by $(\rho, \pi, \rho_b, \dot\rho, \dot\pi, \dot\rho_b)$, while $T^*(T^*\mathcal{Q} \times \mathcal{F}^*) = (\mathcal{Q} \times \mathcal{Q}^* \times \mathcal{F}^*) \times (\mathcal{Q}^* \times \mathcal{Q} \times \mathcal{F})$, with a typical element denoted by $(\rho, \pi, \rho_b, e_\rho, e_\pi, e_b)$. For the duality pairing between $T(T^*\mathcal{Q}\times\mathcal{F}^*)$ and $T^*(T^*\mathcal{Q}\times\mathcal{F}^*)$ we chose

$$\begin{aligned}&\langle(\rho, \pi, \rho_b, e_\rho, e_\pi, e_b), (\rho, \pi, \rho_b, \dot\rho, \dot\pi, \dot\rho_b)\rangle\\ &= \int_M (e_\rho \wedge \dot\rho + e_\pi \wedge \dot\pi) + \int_{\partial M} (e_b \wedge \dot\rho_b + e_b \wedge \operatorname{tr}\dot\rho)\,.\end{aligned} \tag{5.3.1}$$

The choice for this non-degenerate pairing will become clear in Section 5.4.

5.3.1 The Symmetry Group

Let $\mathfrak{G}$ be an Abelian group of $(k-1)$-forms. For any $\alpha \in \mathfrak{G}$ and $\rho \in \mathcal{Q}$, the group $\mathfrak{G}$ action on $\mathcal{Q}$ is

$$\rho \cdot \alpha = \rho + \mathrm{d}\alpha. \tag{5.3.2}$$

This action of gauge group lifts to $T\mathcal{Q} \times \mathcal{F}$ and $T^*\mathcal{Q} \times \mathcal{F}^*$ as $(\rho, \dot\rho, e_b) \cdot \alpha = (\rho + \mathrm{d}\alpha, \dot\rho, e_b)$ and $(\rho, \pi, \rho_b) \cdot \alpha = (\rho + \mathrm{d}\alpha, \pi, \rho_b)$ for $\alpha \in \mathfrak{G}$, $(\rho, \dot\rho, e_b) \in T\mathcal{Q} \times \mathcal{F}$ and $(\rho, \pi, \rho_b) \in T^*\mathcal{Q} \times \mathcal{F}^*$.

The elements of $\mathcal{Q}/\mathfrak{G}$ are equivalence classes $[\rho]$ of k-forms up to exact forms, so that the exterior differential determines a well-defined map from $\mathcal{Q}/\mathfrak{G}$ to $\mathrm{d}\Omega^k$, given by $[\rho] \mapsto \mathrm{d}\rho$, see, e.g., [10]. If the k-th cohomology of M vanishes, we have $\mathcal{Q}/\mathfrak{G} = \mathrm{d}\Omega^k$. Consequently, the quotient $(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*)$ is isomorphic to $\mathcal{Q}/\mathfrak{G} \times \mathcal{Q}^* \times \mathcal{F}^*$, or explicitly

$$T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^* = \mathrm{d}\Omega^k(M) \times \Omega^{n-k}(M) \times \Omega^k(\partial M).$$

The quotient map denoted as $\pi_{\mathfrak{G}} : T^*\mathcal{Q} \times \mathcal{F}^* \to (T^*\mathcal{Q})/\mathfrak{G} \times \mathcal{F}^*$ is given by

$$\pi_{\mathfrak{G}}(\rho, \pi, \rho_b) = (\mathrm{d}\rho, \pi, \rho_b). \tag{5.3.3}$$

Let a representative element of $T^*\mathcal{Q}/\mathfrak{G}\times\mathcal{F}^*$ be $(\bar\rho,\bar\pi,\bar\rho_b)$, with $\bar\rho\in \mathrm{d}\Omega^k(M)$, $\bar\pi\in\Omega^{n-k}(M)$ and $\bar\rho_b\in\Omega^k(\partial M)$. Elements of $T(T^*\mathcal{Q}/\mathfrak{G}\times\mathcal{F}^*)$ will be denoted by $(\bar\rho,\bar\pi,\bar\rho_b,\dot{\bar\rho},\dot{\bar\pi},\dot{\bar\rho}_b)$, while the elements of $T^*(T^*\mathcal{Q}/\mathfrak{G}\times\mathcal{F}^*)$ will be denoted by $(\bar\rho,\bar\pi,\bar\rho_b,\bar e_\rho,\bar e_\pi,\bar e_b)$. The duality pairing is given as

$$\begin{aligned}&\langle(\bar\rho,\bar\pi,\bar\rho_b,\bar e_\rho,\bar e_\pi,\bar e_b),(\bar\rho,\bar\pi,\bar\rho_b,\dot{\bar\rho},\dot{\bar\pi},\dot{\bar\rho}_b)\rangle\\&=\int_M(\bar e_\rho\wedge\dot{\bar\rho}+\bar e_\pi\wedge\dot{\bar\pi})+\int_{\partial M}\bar e_b\wedge\dot{\bar\rho}_b.\end{aligned}\tag{5.3.4}$$

Whenever the base point $(\bar\rho,\bar\pi,\bar\rho_b)$ is clear from the context, we will denote $(\bar\rho,\bar\pi,\bar\rho_b,\dot{\bar\rho},\dot{\bar\pi},\dot{\bar\rho}_b)$ simply by $(\dot{\bar\rho},\dot{\bar\pi},\dot{\bar\rho}_b)$, and similarly $(\bar\rho,\bar\pi,\bar\rho_b,\bar e_\rho,\bar e_\pi,\bar e_b)$ is then denoted by $(\bar e_\rho,\bar e_\pi,\bar e_b)$.

5.3.2 The Reduced Dirac Structure

The generalized canonical Dirac structure is a Poisson structure induced by the linear mapping $\sharp: T^*(T^*\mathcal{Q}\times\mathcal{F}^*)\to T(T^*\mathcal{Q}\times\mathcal{F}^*)$ given by

$$\sharp(\rho,\pi,\rho_b,e_\rho,e_\pi,e_b)=(\rho,\pi,\rho_b,e_\pi,-(-1)^{k(n-k)}e_\rho,-\mathrm{tr}\,e_\pi).\tag{5.3.5}$$

In order to obtain the reduced Poisson structure from the canonical Dirac structure (5.3.5), we need to specify what are the operators $T\pi_{\mathfrak{G}}$ and $T^*\pi_{\mathfrak{G}}$ in the diagram (5.1.4). The space $\mathcal{F}$ is the set of admissible forms $\Omega^{n-k-1}(\partial M)$ that are the traces of $(\mathrm{d}\Omega^k)^*$, as will be made clear in Lemma 5.3.1. Consider an element $(\rho,\pi,\rho_b)\in T^*\mathcal{Q}\times\mathcal{F}^*$, and we recall that $\pi_{\mathfrak{G}}(\rho,\pi,\rho_b)=(\mathrm{d}\rho,\pi,\rho_b)$. Let $T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}: T_{(\rho,\pi,\rho_b)}(T^*\mathcal{Q}\times\mathcal{F}^*)\to T_{(\mathrm{d}\rho,\pi,\rho_b)}(T^*\mathcal{Q}/\mathfrak{G}\times\mathcal{F}^*)$ be the tangent map to $\pi_{\mathfrak{G}}$ at (ρ,π,ρ_b) and consider the cotangent map $T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}: T^*_{(\mathrm{d}\rho,\pi,\rho_b)}(T^*\mathcal{Q}/\mathfrak{G}\times\mathcal{F}^*)\to T^*_{(\rho,\pi,\rho_b)}(T^*\mathcal{Q}\times\mathcal{F}^*)$.

Lemma 5.3.1. *The tangent and cotangent maps $T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}$ and $T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}$ are given by*

$$T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}(\rho,\pi,\rho_b,\dot\rho,\dot\pi,\dot\rho_b)=(\mathrm{d}\rho,\pi,\rho_b,\mathrm{d}\dot\rho,\dot\pi,\dot\rho_b)\tag{5.3.6}$$

and

$$\begin{aligned}&T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}(\mathrm{d}\rho,\pi,\rho_b,\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho)\\&=(\rho,\pi,\rho_b,(-1)^{n-k}\mathrm{d}\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho).\end{aligned}\tag{5.3.7}$$

Proof. The expression (5.3.6) for $T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}$ follows from (5.3.3). To prove (5.3.7), we let $(\dot\rho,\dot\pi,\dot\rho_b)\in T_{(\rho,\pi,\rho_b)}(T^*\mathcal{Q}\times\mathcal{F}^*)$ and consider

$$\begin{aligned}&\left\langle T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}(\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\bar e_\rho),(\dot\rho,\dot\pi,\dot\rho_b)\right\rangle\\&=\left\langle(\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho),T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}(\dot\rho,\dot\pi,\dot\rho_b)\right\rangle\\&=\left\langle(\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho),(\mathrm{d}\dot\rho,\dot\pi,\dot\rho_b)\right\rangle.\end{aligned}$$

Applying Stokes' theorem, we have

$$\begin{aligned}&\left\langle(\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho),(\mathrm{d}\dot\rho,\dot\pi,\dot\rho_b)\right\rangle\\&=\int_M(\bar e_\rho\wedge\mathrm{d}\dot\rho+\bar e_\pi\wedge\dot\pi)+\int_M(-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho\wedge\rho_b-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho\wedge\mathrm{tr}\,\dot\rho)\\&=\int_M((-1)^{n-k}\mathrm{d}\bar e_\rho\wedge\dot\rho+\bar e_\pi\wedge\dot\pi)-\int_{\partial M}(-1)^{n-k}\mathrm{tr}\,\bar e_\rho\wedge\mathrm{tr}\,\dot\rho\,.\end{aligned}$$

Thus, $T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}(\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho)=((-1)^{n-k}\mathrm{d}\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho)$. □

As in the case of a boundaryless manifold [127], the reduced Poisson structure in (5.1.4) is given by

$$[\sharp]_{(\mathrm{d}\rho,\pi,\rho_b)}=T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}\circ\sharp\circ T^*_{(\mathrm{d}\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}$$

for all $(\mathrm{d}\rho,\pi,\rho_b)\in T^*\mathcal{Q}/\mathfrak{G}\times\mathcal{F}^*$.

Theorem 5.3.2. *The reduced Poisson structure is given by*

$$[\sharp](\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho)=(\mathrm{d}\bar e_\pi,-(-1)^{n(k+1)}\mathrm{d}\bar e_\rho,-\mathrm{tr}\,\bar e_\pi)\,.\tag{5.3.8}$$

Proof. Follows from direct calculation of $[\sharp](\bar e_\rho,\bar e_\pi,-(-1)^{n-k}\mathrm{tr}\,\bar e_\rho)$. A similar proof will be given in Section 5.5, but in the discrete context. □

Relation to the Stokes-Dirac structure. The matrix form of the reduced Poisson structure is

$$\begin{pmatrix}\dot{\bar\rho}\\ \dot{\bar\pi}\\ \dot\rho_b\end{pmatrix}=\begin{pmatrix}0&\mathrm{d}&0\\ -(-1)^{n(k+1)}\mathrm{d}&0&0\\ 0&-\mathrm{tr}&0\end{pmatrix}\begin{pmatrix}\bar e_\rho\\ \bar e_\pi\\ (-1)^{n-k}\mathrm{tr}\,\bar e_\rho\end{pmatrix}.\tag{5.3.9}$$

The sign convention in (5.3.9) and the Stokes-Dirac structure (5.2.1) is not the same. To match the signs we introduce new *flow variables* f_p,f_q,f_b

and *effort variables* e_p, e_q, e_b defined as $e_p = \bar{e}_\rho, e_q = (-1)^r \bar{e}_\pi, f_p = \dot{\bar{\rho}}, f_q = (-1)^{n(k+1)+1}\dot{\bar{\pi}}, f_b = -(-1)^r \dot{\bar{\rho}}_b$, where $p = k+1$, $q = n-k$, and $r = pq+1$. With this choice of signs, (5.3.9) becomes

$$\begin{aligned} \begin{pmatrix} f_p \\ f_q \end{pmatrix} &= \begin{pmatrix} 0 & (-1)^r \mathrm{d} \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} e_p \\ e_q \end{pmatrix} \\ f_b &= \operatorname{tr} e_q \\ (-1)^{n-k} \operatorname{tr} e_p &= e_b \,. \end{aligned} \tag{5.3.10}$$

Here, it is important to point out that the boundary effort e_b, unlike in the case of the Stokes-Dirac structure, does not follow from the associate Poisson structure, but rather belongs to the set of admissible derivatives of the flow restricted to the boundary.

5.4 Symmetry in Port-Hamiltonian Systems

Let $t \mapsto (\alpha_{\dot{\rho}}, \alpha_{\dot{\pi}}) \in \Omega^k(M) \times \Omega^{n-k}(M)$ be a time function, and let the Hamiltonian be

$$H(\alpha_{\dot{\rho}}, \alpha_{\dot{\pi}}) = \int_M \mathcal{H}(\mathrm{d}\alpha_{\dot{\rho}}, \alpha_{\dot{\pi}}) \,.$$

It follows that at any time instance $t \in \mathbb{R}$

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \int_M \frac{\delta H}{\delta \alpha_{\dot{\rho}}} \wedge \frac{\partial \alpha_{\dot{\rho}}}{\partial t} + \frac{\delta H}{\delta \alpha_{\dot{\pi}}} \wedge \frac{\partial \alpha_{\dot{\pi}}}{\partial t} + \int_{\partial M} \frac{\partial \mathcal{H}}{\partial (\mathrm{d}\alpha_{\dot{\rho}})} \wedge \frac{\partial \alpha_{\dot{\rho}}}{\partial t} \,.$$

The differential forms $\frac{\partial \alpha_{\dot{\rho}}}{\partial t}, \frac{\partial \alpha_{\dot{\pi}}}{\partial t}$ represent the generalized velocities of the energy variables $\alpha_{\dot{\rho}}, \alpha_{\dot{\pi}}$. The connection with the canonical Dirac structure is made by setting the flows

$$\dot{\rho} = -\frac{\partial \alpha_{\dot{\rho}}}{\partial t} \quad \dot{\pi} = -\frac{\partial \alpha_{\dot{\pi}}}{\partial t} \,,$$

and the efforts

$$e_\rho = \frac{\delta H}{\delta \alpha_{\dot{\rho}}} \,, \quad e_\pi = \frac{\delta H}{\delta \alpha_{\dot{\pi}}} \,.$$

The ***canonical distributed-parameter port-Hamiltonian system*** on an n-dimensional manifold, with the state space $\Omega^k(M) \times \Omega^{n-k}(M)$, the Hamil-

tonian H and the canonical Dirac structure (5.3.5), is given as

$$\begin{aligned}\begin{pmatrix} -\frac{\partial \alpha_{\dot\rho}}{\partial t} \\ -\frac{\partial \alpha_{\dot\pi}}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ -(-1)^{k(n-k)} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta H}{\delta \alpha_{\dot\rho}} \\ \frac{\delta H}{\delta \alpha_{\dot\pi}} \end{pmatrix} \\ \begin{pmatrix} f_b \\ e_b \end{pmatrix} &= \begin{pmatrix} 0 & -\mathrm{tr} \\ -\mathrm{tr} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial (\mathrm{d}\alpha_{\dot\rho})} \\ \frac{\delta H}{\delta \alpha_{\dot\pi}} \end{pmatrix} .\end{aligned} \tag{5.4.1}$$

Proposition 5.4.1. *For the port-Hamiltonian system (5.4.1) the following property*

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \int_{\partial M} e_b \wedge f_b$$

expresses the fact that the increase in energy on the domain M is equal to the power supplied to the system through the boundary ∂M.

Remark 5.4.1. *The system (5.4.1) is precisely the system (2.4.7) on $\mathcal{X} = \Omega^k(M) \times \Omega^{n-k}(M)$, with $G = 0$, $J = -\begin{pmatrix} 0 & 1 \\ (-1)^{k(n-k)} & 0 \end{pmatrix}$, and the natural boundary variables.*

5.4.1 The Reduced Port-Hamiltonian Systems

The Hamiltonian H is invariant if a spatially independent k-form is added to $\alpha_{\dot\rho}$, thus Poisson reduction is applicable. Let the reduced field be $\bar\alpha_{\dot\rho} := \mathrm{d}\alpha_{\dot\rho}$, then the reduced Hamiltonian is

$$H_r(\bar\alpha_{\dot\rho}, \alpha_{\dot\pi}) = \int_M \mathcal{H}_r(\bar\alpha_{\dot\rho}, \alpha_{\dot\pi}) .$$

The port-Hamiltonian system with respect to the reduced Poisson structure is

$$\begin{aligned}\begin{pmatrix} -\frac{\partial \bar\alpha_{\dot\rho}}{\partial t} \\ -\frac{\partial \alpha_{\dot\pi}}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & \mathrm{d} \\ -(-1)^{n(k+1)}\mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta H_r}{\delta \bar\alpha_{\dot\rho}} \\ \frac{\delta H_r}{\delta \alpha_{\dot\pi}} \end{pmatrix} \\ \begin{pmatrix} f_b \\ e_b \end{pmatrix} &= \begin{pmatrix} 0 & -\mathrm{tr} \\ -(-1)^{n-k}\mathrm{tr} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta H_r}{\delta \bar\alpha_{\dot\rho}} \\ \frac{\delta H_r}{\delta \alpha_{\dot\pi}} \end{pmatrix} .\end{aligned} \tag{5.4.2}$$

This is precisely the port-Hamiltonian system given in [98].

We will show how the general considerations of the reduction of port-Hamiltonian systems apply to physical examples of Maxwell's equations and the vibrating string.

5.4.2 Maxwell's Equations

The spatial domain is a three-dimensional Riemannian manifold with boundary. Let ϵ and μ be the electric and the magnetic permeability, and let $*$ be the Hodge star corresponding to the Euclidian metric.

The configuration space $\mathcal{Q}$ is the space of one-forms representing the vector potential A. The group $\mathfrak{G} = \Omega^0(M)$ acts on $\mathcal{Q}$ as

$$f \cdot A = A + \mathrm{d}f\,,$$

with the quotient space $\mathcal{Q}/\mathfrak{G}$ being the space of of magnetic fields $B = \mathrm{d}A$.

The Hamiltonian corresponding to Maxwell's equations is

$$H(A, D) = \frac{1}{2}\int_M (\epsilon^{-1} D \wedge *D + \mu^{-1}\mathrm{d}A \wedge *\mathrm{d}A)$$

and as such is invariant under the gauge symmetry $A \mapsto A + \mathrm{d}f$.

The canonical Hamiltonian equations are

$$\begin{aligned}\begin{pmatrix} -\frac{\partial A}{\partial t} \\ -\frac{\partial D}{\partial t}\end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}\begin{pmatrix} \frac{\delta H}{\delta A} \\ \frac{\delta H}{\delta D}\end{pmatrix} \\ f_b &= \mathrm{tr}(\epsilon^{-1} * D) \\ e_b &= \mathrm{tr}\left(\frac{\partial \mathcal{H}}{\partial(\mathrm{d}A)}\right) = \mathrm{tr}\left(\mu^{-1} * \mathrm{d}A\right)\,,\end{aligned} \tag{5.4.3}$$

where $\frac{\delta H}{\delta D} = *D$ and $\frac{\delta H}{\delta A} = -\mathrm{d} * \mathrm{d}A$.

The energy balance in the case of the unreduced Maxwell's equations takes the form

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \int_{\partial M} \mu^{-1} * \mathrm{d}A \wedge \epsilon^{-1} * D = \int_{\partial M} e_b \wedge f_b\,.$$

The reduced Hamiltonian takes the form

$$H_r(B, D) = \frac{1}{2}\int_M (\epsilon^{-1} D \wedge *D + \mu^{-1} B \wedge *B)\,.$$

The reduced port-Hamiltonian system defined with respect to the Stokes-Dirac structure is

$$\begin{aligned}\begin{pmatrix} -\frac{\partial B}{\partial t} \\ -\frac{\partial D}{\partial t}\end{pmatrix} &= \begin{pmatrix} 0 & \mathrm{d} \\ -\mathrm{d} & 0\end{pmatrix}\begin{pmatrix} *B \\ *D\end{pmatrix} \\ f_b &= \mathrm{tr}(\epsilon^{-1} * D) \\ e_b &= \mathrm{tr}\left(\mu^{-1} * B\right)\,.\end{aligned} \tag{5.4.4}$$

5.4.3 Vibrating String

Consider an elastic string of length l, elasticity modulus T, and mass density μ, subject to traction forces at its ends. The underlying manifold is the segment $M = [0, l] \subset \mathbb{R}$, with coordinate z.

Under the assumption of linear elasticity, the Hamiltonian is given by

$$H(u,p) = \int_M \mathcal{H}(u,p) = \frac{1}{2}\int_M (\mu^{-1} p \wedge *p + T\,\mathrm{d}u \wedge *\mathrm{d}u)\,,$$

where $p \in \Omega^1(M)$ is the momentum conjugate to the displacement $u \in \Omega^0(M)$, and $*$ is the Hodge star.

The canonical Hamiltonian equations are

$$\begin{aligned}
\begin{pmatrix} \frac{\partial u}{\partial t} \\ \frac{\partial p}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta H}{\delta u} \\ \frac{\delta H}{\delta p} \end{pmatrix} \\
f_b &= \mathrm{tr}(*\mu^{-1} p) \\
e_b &= \mathrm{tr}\left(\frac{\partial \mathcal{H}}{\partial(\mathrm{d}u)}\right)\,,
\end{aligned} \tag{5.4.5}$$

or component-wise

$$\begin{aligned}
\frac{\partial u}{\partial t} &= *\mu^{-1} p \\
\frac{\partial p}{\partial t} &= \mathrm{d}(*T\,\mathrm{d}u) \\
f_b &= \mathrm{tr}(*\mu^{-1} p) \\
e_b &= \mathrm{tr}(*T\,\mathrm{d}u)\,.
\end{aligned}$$

The Hamiltonian formulation (5.4.5) is identical to the formulation of the vibrating string in (2.4.11) with the boundary variables given as in (2.4.13). The system (5.4.5) is also mentioned in [103] as the heavy chain system.

The energy balance for the vibrating string is

$$\begin{aligned}
\frac{\mathrm{d}H}{\mathrm{d}t} &= \int_M \frac{\delta H}{\delta u} \wedge \frac{\partial u}{\partial t} + \frac{\delta H}{\delta p} \wedge \frac{\partial p}{\partial t} + \int_{\partial M} \frac{\partial \mathcal{H}}{\partial(\mathrm{d}u)} \wedge \frac{\partial u}{\partial t} \\
&= \int_M -\mathrm{d}(*T\,\mathrm{d}u) \wedge *\mu^{-1} p + *\mu^{-1} p \wedge \mathrm{d}(*T\,\mathrm{d}u) \\
&\quad + \int_{\partial M} *\mu^{-1} p \wedge *T\,\mathrm{d}u \\
&= \int_{\partial M} *\mu^{-1} p \wedge *T\,\mathrm{d}u \\
&= \int_{\partial M} e_b \wedge f_b\,.
\end{aligned}$$

The Hamiltonian is invariant if a time function is added to u. The potential energy can be expressed in terms of the strain $\alpha = \mathrm{d}u$ so that the reduced Hamiltonian is given by

$$H_r(\alpha, p) = \int_M \mathcal{H}_r(u, p) = \frac{1}{2}\int_M (\mu^{-1} p \wedge *p + T\alpha \wedge *\alpha)\,.$$

The Hamiltonian equations of the vibrating string now read as

$$\begin{aligned} \begin{pmatrix} \frac{\partial \alpha}{\partial t} \\ \frac{\partial p}{\partial t} \end{pmatrix} &= \begin{pmatrix} 0 & \mathrm{d} \\ \mathrm{d} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta H_r}{\delta \alpha} \\ \frac{\delta H_r}{\delta p} \end{pmatrix} \\ \begin{pmatrix} f_b \\ e_b \end{pmatrix} &= \begin{pmatrix} 0 & \mathrm{tr} \\ \mathrm{tr} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta H_r}{\delta \alpha} \\ \frac{\delta H_r}{\delta p} \end{pmatrix}\,. \end{aligned} \tag{5.4.6}$$

These are the equations that correspond to the formulation of the vibration string system with respect to the Stokes-Dirac structure that is given in [98].

5.5 Symmetry Reduction in the Discrete Setting

In the discrete world, the configuration space is the set of primal discrete forms $\mathcal{Q} = \Omega^k(K)$ with the dual $\mathcal{Q}^* = \Omega^{n-k}(\star_i K)$. The space of the boundary efforts is $\mathcal{E} = \mathcal{F}^* = \Omega^k(\partial(K))$, and the space of the boundary flows is $\mathcal{F} = \Omega^{n-k-1}(\partial(\star K))$.

Canonical Dirac structure. For the duality pairing between $T(T^*\mathcal{Q} \times \mathcal{F}^*)$ and $T^*(T^*\mathcal{Q} \times \mathcal{F}^*)$ we choose

$$\begin{aligned} &\langle (\rho, \pi, \rho_b, e_\rho, e_\pi, e_b), (\rho, \pi, \rho_b, \dot\rho, \dot\pi, \dot\rho_b)\rangle \\ &\quad = \langle e_\rho \wedge \dot\rho + e_\pi \wedge \dot\pi, K\rangle + \langle e_b \wedge \dot\rho_b, \partial K\rangle, \end{aligned} \tag{5.5.1}$$

where $\wedge$ is the primal-dual wedge product.

The generalized canonical Dirac structure is a Poisson structure induced by the linear mapping $\sharp : T^*(T^*\mathcal{Q} \times \mathcal{F}^*) \to T(T^*\mathcal{Q} \times \mathcal{F}^*)$ given by

$$\begin{aligned} &\sharp(\rho, \pi, \rho_b, e_\rho, e_\pi, e_b) \\ &= (\rho, \pi, \rho_b, e_\pi, -(-1)^{k(n-k)} e_\rho + (-1)^{(k+1)(n-1)} \mathbf{d}_b^{n-k-1} e_b, (-1)^{n-k} \mathbf{tr}^k e_\pi). \end{aligned} \tag{5.5.2}$$

Omitting the base point, the matrix representation of (5.5.2) is

$$\begin{aligned} &\sharp(e_\rho, e_\pi, e_b) \\ &= \begin{pmatrix} 0 & I & 0 \\ -(-1)^{k(n-k)} I & 0 & (-1)^{(k+1)(n-1)} \mathbf{d}_b^{n-k-1} \\ 0 & (-1)^{n-k} \mathbf{tr}^k & 0 \end{pmatrix} \begin{pmatrix} e_\rho \\ e_\pi \\ e_b \end{pmatrix}, \end{aligned}$$

what is an example of generalized canonical Dirac structure.

Symmetry reduction. The group $\mathfrak{G}$ that acts on $\mathcal{Q}$ is described by the following action

$$\alpha \cdot \rho = \rho + \mathbf{d}^{k-1}\alpha$$

for $\alpha \in \mathfrak{G}$ and $\rho \in \mathcal{Q}$, where $\mathbf{d}^{k-1}$ is the discrete exterior derivative.

The quotient is $(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*) = \mathbf{d}^k\Omega^k(K) \times \Omega^{n-k}(\star_i K) \times \Omega^k(\partial(K))$.

As in the continuous setting, the quotient map denoted as $\pi_{\mathfrak{G}} : T^*\mathcal{Q} \times \mathcal{F}^* \to (T^*\mathcal{Q})/\mathfrak{G} \times \mathcal{F}^*$ is given by

$$\pi_{\mathfrak{G}}(\rho, \pi, \rho_b) = (\mathbf{d}^k\rho, \pi, \rho_b). \tag{5.5.3}$$

For the duality pairing between $T^*(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*)$ and $T(T^*\mathcal{Q}/\mathfrak{G} \times \mathcal{F}^*)$, we take

$$\langle(\bar\rho, \bar\pi, \bar{\rho_b}, \bar e_\rho, \bar e_\pi, \bar e_b), (\bar\rho, \bar\pi, \bar{\rho_b}, \dot{\bar\rho}, \dot{\bar\pi}, \dot{\bar{\rho_b}})\rangle = \langle \bar e_\rho \wedge \dot{\bar\rho} + \bar e_\pi \wedge \dot{\bar\pi}, K\rangle + \langle \bar e_b \wedge \dot{\bar{\rho_b}}, \partial K\rangle.$$

As before, whenever the base point $(\bar\rho, \bar\pi, \bar{\rho_b})$ is clear, we will denote $(\bar\rho, \bar\pi, \bar{\rho_b}, \dot{\bar\rho}, \dot{\bar\pi}, \dot{\bar{\rho_b}})$ simply by $(\dot{\bar\rho}, \dot{\bar\pi}, \dot{\bar{\rho_b}})$, and similarly for $(\bar\rho, \bar\pi, \bar{\rho_b}, \bar e_\rho, \bar e_\pi, \bar e_b)$.

Lemma 5.5.1. *The tangent and cotangent maps $T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}$ and $T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}$ are given by*

$$T_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}(\rho, \pi, \rho_b, \dot\rho, \dot\pi, \dot{\rho_b}) = (\mathbf{d}^k\rho, \pi, \rho_b, \mathbf{d}^k\dot\rho, \dot\pi, \dot{\rho_b}) \tag{5.5.4}$$

and

$$T^*_{(\rho,\pi,\rho_b)}\pi_{\mathfrak{G}}(\mathbf{d}^k\rho, \pi, \rho_b, \bar e_\rho, \bar e_\pi, \bar e_b) = (\rho, \pi, \rho_b, (-1)^{n-k}\mathbf{d}_i^{n-k-1}\bar e_\rho, \bar e_\pi, \bar e_b). \tag{5.5.5}$$

Theorem 5.5.2 (Reduced simplicial Dirac structure)**.** *The reduced simplicial Poisson structure is given by*

$$[\sharp](\bar e_\rho, \bar e_\pi, \bar e_b) = \begin{pmatrix} \mathbf{d}^k\bar e_\pi \\ (-1)^{(k+1)(n-1)}(\mathbf{d}_i^{n-k-1}\bar e_\rho + \mathbf{d}_b^{n-k-1}\bar e_b) \\ (-1)^{n-k}\mathbf{tr}^k\bar e_\pi \end{pmatrix}.$$

Proof. To compute the value of $[\sharp](\bar{e}_\rho, \bar{e}_\pi, \bar{e}_b)$ we follow the diagram:

$$
\begin{array}{c}
(\bar{e}_\rho, \bar{e}_\pi, \bar{e}_b) \\
\downarrow T^* \\
\left((-1)^{n-k}\mathbf{d}_i^{n-k-1}\bar{e}_\rho, \bar{e}_\pi, \bar{e}_b\right) \\
\downarrow \sharp \\
\left(\bar{e}_\pi, -(-1)^{(k+1)(n-k)}\left(\mathbf{d}_i^{n-k-1}\bar{e}_\rho + \mathbf{d}_b^{n-k-1}\bar{e}_b\right), (-1)^{n-k}\mathbf{tr}^k\bar{e}_\pi\right) \\
\downarrow T \\
\left(\mathbf{d}^k\bar{e}_\pi, -(-1)^{(k+1)(n-k)}\left(\mathbf{d}_i^{n-k-1}\bar{e}_\rho + \mathbf{d}_b^{n-k-1}\bar{e}_b\right), (-1)^{n-k}\mathbf{tr}^k\bar{e}_\pi\right)
\end{array}
$$

This concludes the proof. □

Port-Hamiltonian systems on a simplicial complex. The canonical port-Hamiltonian system with respect to the canonical Dirac structure is

$$
\begin{aligned}
-\frac{\partial \alpha_{\dot\rho}}{\partial t} &= \frac{\partial H}{\partial \alpha_{\dot\pi}}(\alpha_{\dot\rho}, \alpha_{\dot\pi}) \\
-\frac{\partial \alpha_{\dot\pi}}{\partial t} &= -(-1)^{k(n-1)}\frac{\partial H}{\partial \alpha_{\dot\rho}}(\alpha_{\dot\rho}, \alpha_{\dot\pi}) + (-1)^{(k+1)(n-1)}\mathbf{d}_b^{n-k-1}\bar{e}_b \\
\dot\rho_b &= (-1)^{n-k}\mathbf{tr}^k\frac{\partial H}{\partial \alpha_{\dot\pi}}(\alpha_{\dot\rho}, \alpha_{\dot\pi})\,.
\end{aligned}
\tag{5.5.6}
$$

The rank of the underlying Poison structure is the rank of the symplectic phase space $\Omega^k(K) \times \Omega^{n-k}(\star_i K)$.

The canonical Hamiltonian $(\alpha_{\dot\rho}, \alpha_{\dot\pi}) \mapsto H(\alpha_{\dot\rho}, \alpha_{\dot\pi})$ can be expressed as

$$
H(\alpha_{\dot\rho}, \alpha_{\dot\pi}) := H_r(\mathbf{d}^k\bar{\alpha}_{\dot\rho}, \alpha_{\dot\pi})\,. \tag{5.5.7}
$$

The reduced port-Hamiltonian equations assume the following form

$$
\begin{aligned}
-\frac{\partial \dot\alpha_{\dot\rho}}{\partial t} &= -\mathbf{d}^k\frac{\partial \alpha_{\dot\rho}}{\partial t} = \mathbf{d}^k\frac{\partial H}{\partial \alpha_{\dot\pi}}(\alpha_{\dot\rho}, \alpha_{\dot\pi}) = \mathbf{d}^k\frac{\partial H_r}{\partial \alpha_{\dot\pi}}(\bar{\alpha}_{\dot\rho}, \alpha_{\dot\pi}) \\
-\frac{\partial \alpha_{\dot\pi}}{\partial t} &= -(-1)^{k(n-k)}\frac{\partial H}{\partial \alpha_{\dot\rho}}(\alpha_{\dot\rho}, \alpha_{\dot\pi}) + (-1)^{(k+1)(n-1)}\mathbf{d}_b^{n-k-1}\bar{e}_b \\
&= -(-1)^{(k+1)(n-k)}\left(\mathbf{d}_i^{n-k-1}\frac{\partial H_r}{\partial \bar{\alpha}_{\dot\rho}}(\bar{\alpha}_{\dot\rho}, \alpha_{\dot\pi}) + \mathbf{d}_b^{n-k-1}\bar{e}_b\right) \\
\dot\rho_b &= (-1)^{n-k}\mathbf{tr}^k\frac{\partial H}{\partial \alpha_{\dot\pi}}(\alpha_{\dot\rho}, \alpha_{\dot\pi}) = (-1)^{n-k}\mathbf{tr}^k\frac{\partial H_r}{\partial \alpha_{\dot\pi}}(\bar{\alpha}_{\dot\rho}, \alpha_{\dot\pi})\,,
\end{aligned}
$$

or in the compact matrix form

$$\begin{pmatrix} -\frac{\partial \dot{\alpha}_{\dot{\rho}}}{\partial t} \\ -\frac{\partial \alpha_{\dot{\pi}}}{\partial t} \\ \dot{\rho}_b \end{pmatrix} = \begin{pmatrix} 0 & \mathbf{d}^k & 0 \\ -(-1)^m \mathbf{d}_i^{n-k-1} & 0 & -(-1)^m \mathbf{d}_b^{n-k-1} \\ 0 & (-1)^{n-k} \mathbf{tr}^k & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H_r}{\partial \bar{\alpha}_{\dot{\rho}}} \\ \frac{\partial H_r}{\partial \alpha_{\dot{\pi}}} \\ \bar{e}_b \end{pmatrix}.$$

This is precisely the port-Hamiltonian system on a simplicial manifold as presented in Chapter 4 [110, 109].

5.6 Final Remark

In this chapter I have addressed the issue of the symmetry reduction of the generalized canonical Dirac structure to the Poisson structure associated with the Stokes-Dirac structure. In the discrete world this reduction is pretty standard since the reduced Dirac structure is a Poisson structure. The open avenue for the future work is to find a reduction procedure that would directly lead to the Stokes-Dirac structure. Finding a reduction scheme for other, especially non-constant, Dirac structures is an interesting and open problem.

6

Reaction-Diffusion Systems in the Port-Hamiltonian Framework

> If the Lord Almighty had consulted me before embarking on creation, I should have recommended something simpler.
>
> – Alfonso X of Castile

Reaction-diffusion systems model the evolution of the constituents distributed in space under the influence of chemical reactions and diffusion [117, 123]. These spatially distributed models are essential for the understanding of many important phenomena concerning the development of organisms, coordinated cell behavior, and pattern formation [74]. Guided by the models of reaction-diffusion equations, designing multicellular systems for pattern formation is one of the present research topics in synthetic biology, with application foreseen in tissue engineering, biomaterial fabrication and biosensing [11].

In this chapter I will treat exclusively the effects of diffusion on balanced reaction networks governed by mass action kinetics, though most of the result are valid for any kind of balanced networks. After a brief review of balanced reaction networks closely following the exposition of [101], I will introduce a Dirac structure that captures the geometry of reaction-diffusion systems. We start from the fact that the considered reaction systems are defined with respect to a finite Dirac structure on a manifold. This means that the reaction system from a network modeling perspective can be described by a set of energy-storing elements, a set of energy-dissipating (resistive) elements, and a set of ports (by which the interconnection is modeled), all interconnected by a power-conserving interconnections [96].

From a control and interconnection viewpoint a prime desideratum is to

formulate reaction-diffusion systems with varying boundary conditions in order to allow energy flow through the boundary, since the interaction with the environment takes the place through the boundary. The Stokes-Dirac structure offers a geometric framework for this. Apart from being closed under power-conserving interconnections, it has a property of spatial compositionality, as has been shown in Chapter 2.

It is well-known that adding diffusion to the reaction system can generate behaviors absent in the ode case. This primarily pertains to the problem of diffusion-driven instability which constitutes the basis of Turing's mechanism for pattern formation [124], [75]. Here, the port-Hamiltonian perspective permits us to draw immediately some conclusions regarding passivity of reaction-diffusion systems. In order to apply the Krasovskii-LaSalle principle, we need the precompactness and the global boundedness of classical solution. For this reason, stability analysis seems to be a hard problem. Under certain assumptions in Section 6.5, I will present a result that warrants stability for the asymptotic behavior of the solution of a class of reaction-diffusion systems with Neumann boundary conditions.

In Section 6.7, by adopting a discrete differential geometry-based approach and discretizing the reaction-diffusion system in port-Hamiltonian form, apart from preserving a geometric structure, a compartmental model analogous to the standard one is obtained [54, 56]. Furthermore, I will show asymptotic stability of the compartmental model and verify this result on an example of glycolisis pathway reaction.

Notation. The space of n dimensional real vectors consisting of all strictly positive entries is denoted by $\mathbb{R}^n_+$ and the space of n dimensional real vectors consisting of all nonnegative entries is denoted by $\bar{\mathbb{R}}^n_+$. $\mathbf{1}_m$ denotes a vector of dimension m with all entries equal to 1. The time-derivative $\frac{dx}{dt}(t)$ of a vector x depending on time t will be usually denoted by $\dot{x}$.

Define the mapping $\mathrm{Ln} : \mathbb{R}^m_+ \to \mathbb{R}^m, \quad x \mapsto \mathrm{Ln}(x)$, as the mapping whose i-th component is given by $(\mathrm{Ln}(x))_i := \ln(x_i)$. Similarly, define the mapping $\mathrm{Exp} : \mathbb{R}^m \to \mathbb{R}^m_+, \quad x \mapsto \mathrm{Exp}(x)$, as the mapping whose i-th component is given by $(\mathrm{Exp}(x))_i := \exp(x_i)$. Also, define for any vectors $x, z \in \mathbb{R}^m$ the vector $x \cdot z \in \mathbb{R}^m$ as the element-wise product $(x \cdot z)_i := x_i z_i$, $i = 1, 2, \ldots, m$, and the vector $\frac{x}{z} \in \mathbb{R}^m$ as the element-wise quotient $\left(\frac{x}{z}\right)_i := \frac{x_i}{z_i}$, $i = 1, \cdots, m$. Note that with these notations $\mathrm{Exp}(x + z) = \mathrm{Exp}(x) \cdot \mathrm{Exp}(z)$ and $\mathrm{Ln}(x \cdot z) = \mathrm{Ln}(x) + \mathrm{Ln}(z)$, $\mathrm{Ln}\left(\frac{x}{z}\right) = \mathrm{Ln}(x) - \mathrm{Ln}(z)$.

The space of smooth k-forms in the interior of an n-dimensional manifold M with boundary is $\Omega^k(M)$, while the space of k-forms on ∂M is $\Omega^k(\partial M)$. Define $\Omega^k_m(M) := \Omega^k(M) \times \cdots \times \Omega^k(M)$, with the product being taken m

times. Analogously we define the space $\Omega^k_m(\partial M)$. We will also employ the notion $C^\infty_m(M) := C^\infty(M) \times \cdots \times C^\infty(M)$.

6.1 Introduction

Consider a dynamical system

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x)\,, \quad x \in \mathcal{X} \subseteq \mathbb{R}^m, \quad t \geq 0\,, \tag{6.1.1}$$

where $\mathcal{X}$ is a smooth manifold and $x \mapsto f(x)$ is a smooth vector field. In the present chapter, the dynamical system (6.1.1) is addressed as a reaction system, where the term "reaction" for the moment being is taken in a general, formal sense. A physicochemical interpretation would be that of an open system at mechanical equilibrium involving m reacting constituents with $x_1, \ldots, x_m$ as mass density variables [75]. Later on we will substitute f with a specific vector function.

An important problem in the theory of reaction-diffusion systems is concerned with modeling and describing the effects of adding diffusion to the reaction system [117], [123]. This means that the state x varies from point to point in space and thus (6.1.1) is replaced with a reaction-diffusion system with m structural variables on a n-dimensional smooth manifold M with smooth $(n-1)$-dimensional boundary ∂M. The state-space description of this spatially distributed system is

$$\frac{\partial x}{\partial t} = \operatorname{div}(D(x)\operatorname{grad} x) + f(x)\,, \tag{6.1.2}$$

with $x := (x_1(\xi,t), \ldots, x_m(\xi,t))^{\mathrm{T}} : (M, \mathbb{R}_+) \to \mathcal{X}$, and $x \mapsto D(x) \in \mathbb{R}^{m\times m}$ is a positive-semidefinite diagonal matrix. The operators grad and div act component-wise with respect to the local coordinates $\xi = (\xi_1, \ldots, \xi_n)$. The constraints acting on the system from the outside M impose appropriate boundary conditions. Most frequently these are either Dirichlet conditions

$$x = c_D \quad \text{on} \quad \partial M\,, \tag{6.1.3}$$

or Neumann conditions

$$\operatorname{grad} x \cdot \nu = c_N \quad \text{on} \quad \partial M\,, \tag{6.1.4}$$

where ν is the normal to ∂M, and c_D, c_N are constant vectors. The initial condition of the formulated boundary problem is

$$x(\xi, 0) = x_0(\xi) \quad \text{for} \quad \xi \in M\,, \tag{6.1.5}$$

where x_0 is given.

Three assumption are frequently made concerning this boundary problem [123]:

1. The mapping f is smooth and *bounded* on $\mathcal{X}$.

2. The initial-value problem is well-posed, i.e., for every smooth x_0 the problem (6.1.2)–(6.1.5) possesses a unique solution x, and the semigroup operator, generated by the boundary problem, $S(t) : x_0 \mapsto x(t)$ is smooth for all $t \geq 0$.

3. There exists a closed convex region $\Sigma \subset \mathcal{X}$ which is positively invariant. This means that if $x_0(\xi) \in \Sigma$ for every $\xi \in M$, then $x(\xi, t) \in \Sigma$ for all $t > 0$ for which the solution of (6.1.2)–(6.1.5) exists. For an exhaustive treatment of sufficient or necessary and sufficient conditions on D, f, and Σ, which guarantee the positive invariance of Σ, we refer to [117].

Requiring the smoothness of all the mappings is not necessary and as will be clear from subsequent sections the extension to C^k differentiability (with k as large as the number of derivatives used in the formulas) is immediate. Furthermore, for a class of systems, the second assumption can be relaxed to the case of, say, square integrable functions with the analysis in appropriate Sobolev spaces. The problem, however, is the *boundedness* of f, because the mass action kinetics leads to *polynomial systems*, as will be demonstrated in the forthcoming section.

6.2 Balanced Chemical Reaction Networks

In this section, closely following [101], we revisit the analysis of reversible chemical reactions. Inspired by the recent advances in the network control and graph theory, [101] offers an elegant formulation for the dynamics of reversible chemical reactions. The graph description of the chemical reaction networks considered in [101] has a direct thermodynamical interpretation, which can be regarded as a graph-theoretic version of the formulation derived in the work of Katchalsky, Oster and Perelson [82, 81]. Based on this formulation, it is possible to characterize the space of equilibrium points and provide their dynamical analysis on the state space modulo the space of equilibrium points.

We firstly summarize the mathematical structure of chemical reaction networks. Here, we revisit the work of Horn and Jackson [52, 51] and Feinberg [32, 33] by defining the complexes of a reaction to be the vertices of a graph.

Following [101], these achievements will be formalized in a slightly more abstract manner, also making use of the exposition given in [84]; see also [5] for a nice account.

In Section 6.2.3 we recall the law of mass action kinetics and in Section 6.2.4 we review the framework that describes the dynamics of reversible chemical reaction networks. The resulting form of the dynamical equations for balanced reaction networks will be fundamental to the analysis throughout the chapter.

Finally, we call back to our attention results that characterize the set of equilibria of a balanced chemical reaction network and show their asymptotic stability.

6.2.1 Stoichiometry

Consider a chemical reaction network involving m chemical species (metabolites), among which r chemical reactions take place. The basic structure underlying the dynamics of the vector $x \in \bar{\mathbb{R}}^m_+$ of concentrations $x_i, i = 1, \ldots, m$, of the chemical species is given by the *balance laws*

$$\dot{x} = Sv, \tag{6.2.1}$$

where S is an $m \times r$ matrix, called the ***stoichiometric matrix***. The elements of the vector $v \in \mathbb{R}^r$ are commonly called the (reaction) *fluxes*. The stoichiometric matrix S, which consists of (positive and negative) integer elements, captures the basic conservation laws of the reactions.

6.2.2 The Complex Graph

The network structure of a chemical reaction network cannot be directly captured by a graph involving the chemical species, because, in general, there are more than two species involved in a reaction. Following the approach originating in the work of Horn and Jackson [52, 51] and Feinberg [32, 33], we will introduce the space of ***complexes***. The set of complexes of a chemical reaction network is simply defined as the union of all the different left- and right-hand sides (substrates and products) of the reactions in the network. The expression of the complexes in terms of the chemical species is formalized by an $m \times c$ matrix Z, whose ρ-th column captures the expression of the ρ-th complex in the m chemical species.

Since the complexes are left- and right-hand sides of the reactions they can be naturally associated with the vertices of a *directed graph*, with edges corresponding to the reactions. The complexes on the left-hand side of the reactions are called the *substrate* complexes and those on the right-hand side of

the reactions are called the *product* complexes. Formally, the reaction $\sigma \rightleftharpoons \pi$ between the σ-th and the π-th complex defines a directed edge with tail vertex being the σ-th complex and head vertex being the π-th complex. The resulting graph is called the *complex graph*.

Any directed graph is defined by its ***incidence matrix*** B. This is an $c \times r$ matrix, c being the number of vertices and r being the number of edges, with (ρ, j)-th element equal to -1 if vertex ρ is the tail vertex of edge j and 1 if vertex ρ is the head vertex of edge j, while 0 otherwise (see, for instance, [14]). There is a close relation between the matrix Z and the stoichiometric matrix S, which is expressed as $S = ZB$, with B being the incidence matrix of the complex graph. For this reason we will call Z the ***complex stoichiometric matrix***. Hence the relation $\dot{x} = Sv$ between the fluxes v through the chemical reaction network and the time-derivative of vector of chemical species x can be also written as $\dot{x} = ZBv$, with the vector Bv belonging to the space of complexes $\mathbb{R}^c$.

6.2.3 The General Form of Mass Action Kinetics

The evolution of the state vector x is given once the internal fluxes v are specified as a function $v = v(x)$ of x, defining the *reaction rates*. The most basic model for specifying the reaction rates is ***mass action kinetics***. For a reversible reaction network with r reactions, the mass action rate of the n-th reactions with a substrate complex $\mathcal{S}$ and a product complex $\mathcal{P}$ is given by

$$v_j(x) = k_j^{\text{forw}} \prod_{i=1}^{m} x_i^{Z_{i\mathcal{S}_j}} - k_j^{\text{rev}} \prod_{i=1}^{m} x_i^{Z_{i\mathcal{P}_j}}, \tag{6.2.2}$$

where $Z_{i\rho}$ is the (i, ρ)-th element of the complex stoichiometric matrix Z, and $k_j^{\text{forw}}, k_j^{\text{rev}} \geq 0$ are the forward/reverse reaction constants of the j-th reaction, respectively. Without loss of generality we will throughout assume that for every j the constants $k_j^{\text{forw}}, k_j^{\text{rev}}$ are *not both equal to zero* (since in this case the j-th reaction is not active).

Let $Z_{\mathcal{S}_j}$ and $Z_{\mathcal{P}_j}$ denote the columns of the complex stoichiometry matrix Z corresponding to the substrate and the product complexes of the j-th reaction. The mass action reaction equation (6.2.2) for the j-th reaction from substrate complex $\mathcal{S}_j$ to product complex $\mathcal{P}_j$ can be rewritten as

$$v_j(x) = k_j^{\text{forw}} \exp\left(Z_{\mathcal{S}_j}^{\mathrm{T}} \mathrm{Ln}(x)\right) - k_j^{\text{rev}} \exp\left(Z_{\mathcal{P}_j}^{\mathrm{T}} \mathrm{Ln}(x)\right). \tag{6.2.3}$$

Let the mass action rate for the complete set of reactions be given by the vector $v(x) = \begin{bmatrix} v_1(x) & \cdots & v_r(x) \end{bmatrix}^{\mathrm{T}}$. For every $\sigma, \pi \in \{1, \ldots, c\}$, denote by $a_{\sigma\pi} =$

k_j^{rev}, $a_{\pi\sigma} = k_j^{\text{forw}}$ if $(\sigma, \pi) = (\mathcal{S}_j, \mathcal{P}_j)$, $j \in \{1, \ldots, r\}$ and $a_{\sigma\pi} = 0$ elsewhere. Define the *weighted adjacency matrix* A of the complex graph as the matrix with (σ, π)-th element $a_{\sigma\pi}$, where $\sigma, \pi \in \{1, \ldots, c\}$. Furthermore, define the *weighted Laplacian* matrix L as the $c \times c$ matrix $L := \Delta - A$, where Δ is the diagonal matrix whose (ρ, ρ)-th element is equal to the sum of the elements of the ρ-th column of A. Then it can be verified that the vector $Bv(x)$ for the mass action reaction rate vector $v(x)$ is equal to $Bv(x) = -L\text{Exp}\left(Z^{\text{T}}\text{Ln}(x)\right)$. Hence the dynamics can be compactly written as

$$\dot{x} = -ZL\text{Exp}\left(Z^{\text{T}}\text{Ln}(x)\right). \tag{6.2.4}$$

Here it needs to be noted that a similar expression of the dynamics corresponding to mass action kinetics, in less explicit form, was already obtained in [118].

6.2.4 Balanced Mass Action Kinetics

A vector of concentrations $x^* \in \mathbb{R}^m_+$ is called an *equilibrium* for the dynamics $\dot{x} = Sv(x)$ if $Sv(x^*) = 0$. Furthermore, $x^* \in \mathbb{R}^m_+$ is called a ***thermodynamic equilibrium*** if $v(x^*) = 0$. Clearly, any thermodynamic equilibrium is an equilibrium, but not necessarily the other way around (since in general $S = ZB$ is not injective).

Consider the j-th reaction from substrate $\mathcal{S}_j$ to product $\mathcal{P}_j$, described by the mass action rate equation

$$v_j(x) = k_j^{\text{forw}} \exp\left(Z_{\mathcal{S}_j}^{\text{T}}\text{Ln}(x)\right) - k_j^{\text{rev}} \exp\left(Z_{\mathcal{P}_j}^{\text{T}}\text{Ln}(x)\right).$$

Then $x^* \in \mathbb{R}^m_+$ is a thermodynamic equilibrium, i.e., $v(x^*) = 0$, if and only if

$$\kappa_j(x^*) := k_j^{\text{forw}} \exp\left(Z_{\mathcal{S}_j}^{\text{T}}\text{Ln}(x^*)\right) = k_j^{\text{rev}} \exp\left(Z_{\mathcal{P}_j}^{\text{T}}\text{Ln}(x^*)\right),\ j = 1, \cdots, r. \tag{6.2.5}$$

The mass action reaction rate of the j-th reaction now can be written as

$$v_j(x) = \kappa_j(x^*)\left(\exp\left(Z_{\mathcal{S}_j}^{\text{T}}\text{Ln}\left(\frac{x}{x^*}\right)\right) - \exp\left(Z_{\mathcal{P}_j}^{\text{T}}\text{Ln}\left(\frac{x}{x^*}\right)\right)\right),$$

where for any vectors $x, z \in \mathbb{R}^m$ the quotient vector $\frac{x}{z} \in \mathbb{R}^m$ is defined elementwise. Defining the $r \times r$ diagonal matrix of balanced reaction constants as

$$\mathcal{K}(x^*) := \text{diag}\big(\kappa_1(x^*), \cdots, \kappa_r(x^*)\big), \tag{6.2.6}$$

it follows that the mass action reaction rate vector of a balanced reaction network can be written as

$$v(x) = -\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right)\right),$$

and thus the dynamics of a ***balanced reaction network*** takes the form

$$\dot{x} = -ZB\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right)\right), \quad \mathcal{K}(x^*) > 0. \tag{6.2.7}$$

This form will be the starting point for the analysis of balanced chemical reaction networks in the rest of this chapter.

Furthermore, we shall assume the validity of the ***global persistency conjecture,*** which states that for any positive initial condition $x_0 \in \mathbb{R}^m_+$, the solution $t \mapsto x(t)$ of (6.2.7) satisfies: $\liminf_{t\to\infty} x(t) > 0$. The global persistency conjecture recently was proven for the single linkage class case in [3], but for the system (6.2.7) remains an *open problem.*

The matrix $B\mathcal{K}(x^*)B^{\mathrm{T}}$ in (6.2.7) again defines a *weighted Laplacian* matrix for the complex graph, with weights given by the balanced reaction constants $\kappa_1(x^*), \ldots, \kappa_r(x^*)$. Note that this is in general a *different* weighted Laplacian matrix than the one obtained before. In particular, a main difference is that the weighted Laplacian $B\mathcal{K}(x^*)B^{\mathrm{T}}$ is necessarily *symmetric.* Among others, cf. [14], this implies that the Laplacian $B\mathcal{K}(x^*)B^{\mathrm{T}}$ is in fact independent of the *orientation* of the graph. Thus we may replace any reaction $\mathcal{S} \rightleftharpoons \mathcal{P}$ by $\mathcal{P} \rightleftharpoons \mathcal{S}$ without altering the Laplacian $B\mathcal{K}(x^*)B^{\mathrm{T}}$, in agreement with the usual understanding of a reversible reaction network. The symmetrization of the Laplacian has been accomplished by the modification of $\mathrm{Ln}(x)$ into $\mathrm{Ln}\left(\frac{x}{x^*}\right)$, and using the assumption that x^* is a thermodynamic equilibrium.

Note that $\mathcal{K}(x^*)$, and therefore the Laplacian matrix $B\mathcal{K}(x^*)B^{\mathrm{T}}$, is in principle *dependent* on the choice of the thermodynamic equilibrium x^*. In [101] the authors showed that actually this dependence is minor: for a connected complex graph the matrix $\mathcal{K}(x^*)$ is, *up to a positive multiplicative factor*, independent of the choice of the thermodynamic equilibrium x^* (see Section 3.3 in [101]).

It also follows that once a thermodynamic equilibrium x^* is given, the set of *all* thermodynamic equilibria is described by the following proposition.

Proposition 6.2.1 ([101])**.** *Let $x^* \in \mathbb{R}^m_+$ be a thermodynamic equilibrium, then the set of all thermodynamic equilibria is given by*

$$\mathcal{E} := \{x^{**} \in \mathbb{R}^m_+ \mid S^{\mathrm{T}}\mathrm{Ln}\,(x^{**}) = S^{\mathrm{T}}\mathrm{Ln}\,(x^*)\}. \tag{6.2.8}$$

6.2.5 Stability of Balanced Reaction Networks

Let us define, up to a constant, $\mu(x) := \mathrm{Ln}\left(\frac{x}{x^*}\right)$ as the chemical potential vector and the Gibbs' free energy

$$G(x) = x^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right) + (x^* - x)^{\mathrm{T}}\,\mathbf{1}_m, \tag{6.2.9}$$

where $\mathbf{1}_m$ denotes a vector of dimension m with all ones. It can be immediately checked that

$$\frac{\partial G}{\partial x}(x) = \mathrm{Ln}\left(\frac{x}{x^*}\right) = \mu(x).$$

It follows that the equations of a balanced chemical reaction network (6.2.7) can be equivalently written as

$$\dot{x} = -ZB\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\frac{\partial G}{\partial x}(x)\right), \quad \mu(x) = \frac{\partial G}{\partial x}(x). \tag{6.2.10}$$

In [101] the function $x \mapsto G(x)$ was employed as a *Lyapunov function* for the chemical reaction network. In particular the authors showed that G is non-increasing along solution trajectories.

Remark 6.2.1 ([101])**.** *Note that the definition of G depends on the chosen thermodynamical equilibrium. Denoting the functions for different thermodynamic equilibria x^* and x^{**} by G^*, respectively G^{**}, it is seen that $G^{**}(x) = G^*(x) + x^{\mathrm{T}}(\mathrm{Ln}(x^*) - \mathrm{Ln}(x^{**})) + (x^{**} - x^*)^{\mathrm{T}}\mathbf{1}_m$.*

Making use of the formulation of the dynamics of balanced reaction networks in (6.2.7), in [101] it was shown that all equilibria of a balanced reaction network are actually thermodynamic equilibria, and thus given by (6.2.8). A similar result was obtained in the classical papers [51, 52, 33] for a different class of chemical reaction networks (roughly speaking, weakly reversible networks of deficiency zero or deficiency one under additional conditions).

Theorem 6.2.2 ([101])**.** *Consider a balanced chemical reaction network $\dot{x} = Sv = ZBv$ with m species and r reactions governed by mass action kinetics, with thermodynamic equilibrium x^*, i.e., $v(x^*) = 0$, described as in (6.2.7). Then the set of all equilibria is equal to the set $\mathcal{E} := \{x^{**} \in \mathbb{R}^m_+ \mid S^T\mathrm{Ln}(x^{**}) = S^{\mathrm{T}}\mathrm{Ln}(x^*) = 0\}$ of thermodynamic equilibria given in (6.2.8).*

The function G serves as a Lyapunov function for (6.2.7) to assert global asymptotic stability of the set of equilibria $\mathcal{E}$.

Theorem 6.2.3 ([101]). *Consider a balanced mass action reaction network given by (6.2.7) or, equivalently, by (6.2.10). Then for every initial condition $x(0) \in \mathbb{R}^m_+$, the species concentration x converges for $t \to \infty$ to $\mathcal{E}$.*

In the remaining of this chapter, we will extend some of the results of balanced chemical reaction networks to spatially distributed systems.

6.3 Geometric Formulation

The Stokes-Dirac structure for reaction-diffusion systems employed in this thesis will be defined on the space of differential forms on a Riemannian manifold with boundary. The geometric content of the involved physical (chemical, etc.) variables is expressed by identifying them as differential k-forms, for appropriate k. This interpretation, as we have seen in the previous chapters, is ubiquitous in the case of Maxwell's equation, the telegraph equations, and many other electrical and electromechanical systems, but in the case of reaction-diffusion systems this interpretation is far less-known.

6.3.1 Exterior Formulation

The formulation of a reaction-diffusion system as a port-Hamiltonian system on a *compact* n-dimensional smooth *Riemannian* manifold M with boundary ∂M is given as follows. We identify the mass density variables with an m component vector of 0-forms, that is $x \in \Omega^0_m(M)$. The influence of the external world (reaction-diffusion system) to the system (outside world) is modeled through the efforts $e_b \in \Omega^0_m(\partial M)$ (and flows $f_b \in \Omega^{n-1}_m(\partial M)$). The reaction part is in its nature finite-dimensional and as such is modeled as the interconnection of the atomic elements, each of them characterized by a particular energetic behavior (energy storing, energy conversion or dissipation). Each of these elements can interact with the environment by means of a port—a couple of inputs and outputs whose combination gives the power flow. The geometric content of the reaction part is captured by a standard Dirac structure. The transport of the constituents in space is governed by the laws of diffusion, which is modeled as a thermal damping by termination of the appropriate ports (see Figure 6.1). The picture for this choice of variables will become clear later on.

Let the space of flows be $\mathcal{F}$ and its dual the space of efforts be $\mathcal{E} = \mathcal{F}^*$. We set $\mathcal{F} := \mathcal{F}_x \oplus \mathcal{F}_d \oplus \mathcal{F}_r \oplus \mathcal{F}_b$, where $\mathcal{F}_x = \Omega^0_m(M)$ is the carrier space of concentrations, $\mathcal{F}_d = \Omega^1_m(M)$ the space of gradients, $\mathcal{F}_r = \Omega^0_m(M)$ the reaction flows, and $\mathcal{F}_b = \Omega^{n-1}_m(\partial M)$ being the space of boundary fluxes. In the interior

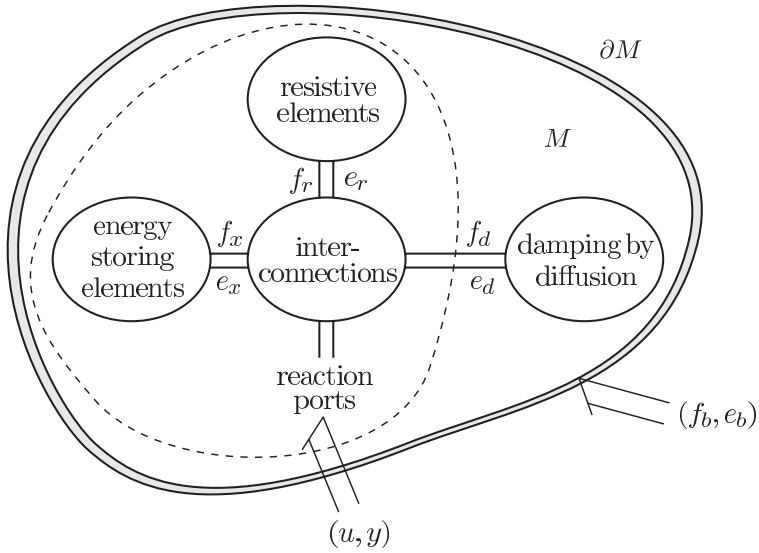


Figure 6.1: Reaction-diffusion system as a dissipative distributed port-Hamiltonian system. The conjugate variables u and y represent the inflows and the outflows of the reaction dynamics. In this thesis, the reaction system is considered to be closed; that is, either $u = 0$ or $y = 0$.

of the domain M, there is a natural identification of k and $(n-k)$ forms via the Hodge star operator. The space of efforts is defined as $\mathcal{E} := \mathcal{E}_x \oplus \mathcal{E}_d \oplus \mathcal{E}_r \oplus \mathcal{E}_b$, with $\mathcal{E}_x = \Omega^0_m(M)$, $\mathcal{E}_d = \Omega^1_m(M)$, $\mathcal{E}_r = \Omega^0_m(M)$, and $\mathcal{E}_b = \Omega^0_m(\partial M)$.

A non-degenerate pairing between $\mathcal{F}$ and $\mathcal{E}$ is defined by the following bilinear form on $\mathcal{F} \times \mathcal{E}$ with values in $\mathbb{R}$

$$\begin{aligned}
&\langle\!\langle (f^1_x, f^1_d, f^1_\gamma, f^1_b, e^1_x, e^1_d, e^1_r, e^1_b), (f^2_x, f^2_d, f^2_r, f^2_b, e^2_x, e^2_d, e^2_r, e^2_b) \rangle\!\rangle \\
&\quad := \left\langle f^1_x, e^2_x \right\rangle_{L^2\Omega^0_m} + \left\langle f^1_d, e^2_d \right\rangle_{L^2\Omega^1_m} + \left\langle f^1_r, e^2_r \right\rangle_{L^2\Omega^0_m} \\
&\qquad + \left\langle f^2_x, e^1_x \right\rangle_{L^2\Omega^0_m} + \left\langle f^2_d, e^1_d \right\rangle_{L^2\Omega^1_m} + \left\langle f^2_r, e^1_r \right\rangle_{L^2\Omega^0_m} \\
&\qquad + \int_{\partial Z} \left(f^1_b \wedge e^2_b + f^2_b \wedge e^1_b \right) ,
\end{aligned} \tag{6.3.1}$$

where $(f^i_x, f^i_d, f^i_r, f^i_b) \in \mathcal{F}$ and $(e^i_x, e^i_d, e^i_r, e^i_b) \in \mathcal{E}$, $i = 1, 2$. The inner product in $\Omega^k_m(M)$ is given by

$$\langle \alpha, \beta \rangle_{L^2\Omega^k_m} = \int_M \alpha \wedge * \beta, \quad \alpha,\, \beta \in \Omega^k_m(M),$$

where the Hodge star $*$ and the wedge product act component-wise.

The Stokes-Dirac structure that underpins the geometry of reaction-diffusion systems is a maximally isotropic subbundle of $\mathcal{F} \times \mathcal{E}$. The following theorem gives the construction of a such Dirac structure.

Theorem 6.3.1. *Define* $\mathcal{D} \subset \mathcal{F} \times \mathcal{E}$ *by*

$$\begin{aligned} \mathcal{D} := \big\{ (f_x, f_d, f_r, f_b, e_x, e_d, e_r, e_b) \in \mathcal{F} \times \mathcal{E} \,\big|\, & \\ \begin{pmatrix} f_x \\ f_d \\ e_r \end{pmatrix} &= \begin{pmatrix} 0 & -\delta & -Z \\ \mathrm{d} & 0 & 0 \\ Z^{\mathrm{T}} & 0 & 0 \end{pmatrix} \begin{pmatrix} e_x \\ e_d \\ f_r \end{pmatrix}, \\ \begin{pmatrix} e_b \\ f_b \end{pmatrix} &= \begin{pmatrix} \mathrm{tr} & 0 & 0 \\ 0 & \mathrm{tr}* & 0 \end{pmatrix} \begin{pmatrix} e_x \\ e_d \\ f_r \end{pmatrix} \big\}, \end{aligned} \tag{6.3.2}$$

where Z *is an* $m \times c$ *matrix,* d *is the exterior derivative,* δ *is the codifferential operator,* $*$ *is the Hodge star, and* tr *is the trace on the boundary* ∂M*. The subbundle* $\mathcal{D}$ *is a Dirac structure with respect to the bilinear form* $\langle\langle , \rangle\rangle$*.*

Proof. Using the fact that $\langle Z f_r, e_x \rangle_{L^2\Omega^0_m} = \langle f_r, Z^{\mathrm{T}} e_x \rangle_{L^2\Omega^0_m}$ for any $f_r \in \Omega^0_m(M)$ and $e_x \in \Omega^0_m(M)$, and applying the integration by parts formula

$$\langle \mathrm{d} e_x, e_d \rangle_{L^2\Omega^1_m} = \langle e_x, \delta e_d \rangle_{L^2\Omega^0_m} + \int_{\partial M} \mathrm{tr}\, e_x \wedge \mathrm{tr}(* e_d),$$

for $e_x \in \Omega^0_m(M),\ e_d \in \Omega^1_m(M)$, similar to Theorem 2.3.4, it can be shown that $\mathcal{D} = \mathcal{D}^{\perp}$. □

6.3.2 Vector Calculus Formulation

Because the manifold M is equipped with a Riemannian metric, it is possible to identify each 0-form and n-form with a scalar valued function. Also, each 1-form and $(n-1)$-form can be identified with a vector field. The associated fields are called proxy fields for the differential forms. This means that the space $\Omega^1(M)$ and $\Omega^{n-1}(M)$ are identified with the space $C^\infty(M; \mathbb{R}^n)$.

Interpreted in terms of the proxy fields, the exterior derivative operators $\mathrm{d} : \Omega^0(M) \to \Omega^1(M)$ and $\mathrm{d} : \Omega^{n-1}(M) \to \Omega^n(M)$ become $\mathrm{grad} : C^\infty(M) \to C^\infty(M; \mathbb{R}^n)$ and $\mathrm{div} : C^\infty(M; \mathbb{R}^n) \to C^\infty(M)$. In the similar manner, the codifferential operator $\delta : \Omega^1(M) \to \Omega^0(M)$ becomes $-\mathrm{div} : C^\infty(M; \mathbb{R}^n) \to C^\infty(M)$.

The trace operation on 0-forms is just the restriction to the boundary, and for a $(n-1)$-form f, the trace corresponds to the scalar $f \cdot \nu$ (with ν the unit

normal) at each boundary point. For more details confer to Chapter 2 or see, for instance, [8].

Now, the flows and the efforts space can be identified such that $\mathcal{F}_x = \mathcal{E}_x = C^\infty_m(M)$, $\mathcal{F}_d = \mathcal{E}_d = C^\infty_m(M;\mathbb{R}^n)$, $\mathcal{F}_r = \mathcal{E}_r = C^\infty_m(M)$, and $\mathcal{F}_b = \mathcal{E}_b = C^\infty_m(\partial M)$. Furthermore, $\mathcal{F} = \mathcal{E} = \mathcal{F}_x \oplus \mathcal{F}_d \oplus \mathcal{F}_r \oplus \mathcal{F}_b$.

The inner product in $C^\infty_m(M)$ is given by

$$\langle \alpha, \beta \rangle_{L^2_m(M)} = \int_M \alpha^{\mathrm{T}}(\xi)\beta(\xi)\mathrm{d}\xi, \quad \alpha,\, \beta \in C^\infty_m(M),$$

where $\mathrm{d}\xi := \mathrm{d}\xi^1 \wedge \cdots \wedge \mathrm{d}\xi^n$ is the volume element on M. Similarly, the inner product on the boundary ∂M is defined by

$$\langle \alpha, \beta \rangle_{L^2_m(\partial M)} = \int_{\partial M} \alpha^{\mathrm{T}}(\xi)\beta(\xi)\mathrm{d}\xi_A, \quad \alpha,\, \beta \in C^\infty_m(\partial M),$$

where $\mathrm{d}\xi_A := \mathrm{d}\xi^1 \wedge \cdots \wedge \mathrm{d}\xi^{n-1}$ is the volume form on the boundary ∂M. Analogously, we defined the inner product in $C^\infty_m(M;\mathbb{R}^n)$ and $C^\infty_m(\partial M;\mathbb{R}^{n-1})$.

The proxy representation of (6.3.1) is

$$\begin{aligned}
&\langle\!\langle (f^1_x, f^1_d, f^1_\gamma, f^1_b, e^1_x, e^1_d, e^1_r, e^1_b), (f^2_x, f^2_d, f^2_r, f^2_b, e^2_x, e^2_d, e^2_r, e^2_b) \rangle\!\rangle \\
&\quad := \left\langle f^1_x, e^2_x \right\rangle_{L^2_m(M)} + \left\langle f^1_d, e^2_d \right\rangle_{L^2_m(M)} + \left\langle f^1_r, e^2_r \right\rangle_{L^2_m(M)} \\
&\qquad + \left\langle f^2_x, e^1_x \right\rangle_{L^2_m(M)} + \left\langle f^2_d, e^1_d \right\rangle_{L^2_m(M)} + \left\langle f^2_r, e^1_r \right\rangle_{L^2_m(M)} \\
&\qquad + \left\langle f^1_b, e^2_b \right\rangle_{L^2_m(\partial M)} + \left\langle f^2_b, e^1_b \right\rangle_{L^2_m(\partial M)},
\end{aligned}$$

where $(f^i_x, f^i_d, f^i_r, f^i_b) \in \mathcal{F}$ and $(e^i_x, e^i_d, e^i_r, e^i_b) \in \mathcal{E}$, $i = 1, 2$.

The subspace $\mathcal{D} \subset \mathcal{F} \times \mathcal{E}$ specified by

$$\begin{aligned}
\mathcal{D} = \Big\{ &(f_x, f_d, f_r, f_b, e_x, e_d, e_r, e_b) \in \mathcal{F} \times \mathcal{E} \,\big|\, \\
&f_x = \operatorname{div} e_d - Z f_r \text{ and } f_d = \operatorname{grad} e_x \text{ and } e_r = Z^{\mathrm{T}} e_x \ \text{ in } \ M, \\
&e_b = \operatorname{tr} e_x \text{ and } f_b = \nu \cdot \operatorname{tr} e_d \ \text{ on } \ \partial M \Big\},
\end{aligned} \tag{6.3.3}$$

a *Dirac structure* with respect to the proxy bilinear form $\langle\!\langle , \rangle\!\rangle$.

6.4 Reaction-Diffusion Dynamics

In order to obtain port-Hamiltonian formulation of reaction-diffusion system, we define the energy storage relations

$$f_x = -\frac{\partial x}{\partial t}, \qquad e_x = \frac{\partial G}{\partial x}(x), \tag{6.4.1}$$

where G is the Hamiltonian (Gibbs' free energy associated with the reaction system), while the energy of reaction-diffusion system is $\mathcal{G} = \int_M G \mathrm{d}\xi$, with $\mathrm{d}\xi$ being the standard volume form.

The power-dissipation of the reaction part is

$$f_r = -B\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}(e_r)\,, \tag{6.4.2}$$

where the mapping $B\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}(\cdot)$ satisfies

$$e_r^{\mathrm{T}} f_r \leq 0 \quad \text{for all} \quad e_r \in \mathcal{E}_r\,. \tag{6.4.3}$$

This is due to the fact that the exponential function is strictly increasing, so

$$\begin{aligned}\gamma^{\mathrm{T}}B\mathcal{K}B^{\mathrm{T}}\mathrm{Exp}(\gamma) &= \sum_{j=1}^{r}\left(\gamma_{\mathcal{P}_j}(x) - \gamma_{\mathcal{S}_j}(x)\right)\left(\exp\left(\gamma_{\mathcal{P}_j}(x)\right) - \exp\left(\gamma_{\mathcal{S}_j}(x)\right)\right)\kappa_j(x^*)\\ &\geq 0\end{aligned}$$

for $\kappa_j(x^*) > 0$, $j = 1, \ldots, r$.

Ordinarily, diffusion is treated as power-dissipation by thermal motion of particles and as such quantitatively is characterized by the diffusion matrix D introduced in (6.1.2), which explicitly refers to the state variable x. In the work at hand diffusion is modeled by termination of the diffusion port as

$$e_d = -\mathcal{R}_d(f_d)\,, \tag{6.4.4}$$

where $\mathcal{R}_d : \mathcal{F}_d \to \mathcal{E}_d$ is in general a nonlinear mapping satisfying the dissipation inequality

$$e_d^{\mathrm{T}} f_d \leq 0 \quad \text{for all} \quad f_d \in \mathcal{F}_d\,.$$

The operator $\mathcal{R}_d$, instead of acting upon the state x, acts upon its gradient and takes the gradient of the co-energy variable as its argument (i.e., the chemical potential μ). We call this operator the energy-diffusion operator.

When the energy-diffusion operator $\mathcal{R}_d$ is a matrix function of the state x, these constitutive relations define the reaction-diffusion system in the port-Hamiltonian framework as

$$\begin{aligned}\frac{\partial x}{\partial t} &= \mathrm{div}\Big(\mathcal{R}_d(x)\mathrm{grad}\,\mathrm{Ln}\left(\frac{x}{x^*}\right)\Big) - ZB\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right)\right)\\ e_b &= \mathrm{Ln}\left(\frac{x}{x^*}\right)|_{\partial M}\\ f_b &= \mathcal{R}_d(x)\mathrm{grad}\,\mathrm{Ln}\left(\frac{x}{x^*}\right)\cdot\nu|_{\partial M}\,,\end{aligned} \tag{6.4.5}$$

with the Gibbs' free energy associated with the reaction system being $G(x) = x^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right) + (x^* - x)^{\mathrm{T}}\mathbf{1}_m$ for $x \in C^\infty_m(M)$, while the total energy of reaction-diffusion system is $\mathcal{G} = \int_M G\mathrm{d}\xi$

Because $\mathrm{grad}\,\mathrm{Ln}\left(\frac{x}{x^*}\right) = \mathrm{diag}\left(\frac{1}{x_1}, \ldots, \frac{1}{x_m}\right)\mathrm{grad}\,x$, the system (6.4.5) is in the form (6.1.2) with $\mathcal{R}_d(x) = \mathrm{diag}\,(x_1, \ldots, x_m)\,D(x)$ and the reaction dynamics $f(x) = -ZB\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right)\right)$.

Stnadard model. The dynamical analysis of the balanced reaction networks presented in [101] is given on the state space modulo the space of equilibrium points. For the sake of thermodynamical consistency, we rewrite the system (6.4.5) into the form given in terms of the disagreement vector $\frac{x}{x^*}$ as

$$\begin{aligned}
\frac{\partial x}{\partial t} &= \mathrm{div}\Big(R_d(x)\mathrm{grad}\Big(\frac{x}{x^*}\Big)\Big) - ZB\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right)\right)\\
e_b &= \mathrm{Ln}\left(\frac{x}{x^*}\right)|_{\partial M}\\
f_b &= R_d(x)\mathrm{grad}\Big(\frac{x}{x^*}\Big)\cdot\nu|_{\partial M}\,,
\end{aligned} \tag{6.4.6}$$

where $R_d(x) := \mathcal{R}_d(x)\mathrm{diag}\left(\frac{x_1^*}{x_1}, \ldots, \frac{x_m^*}{x_m}\right)$.

The existence of solutions for the systems (6.4.5) and (6.4.6) is a complex issue. The extensive literature dealing with nonlinear reaction-diffusion systems [117, 123, 91] *does not* provide a result which will warrant the existence of a solution in some sense. In the forthcoming section I will address this problem for the class with $R_d(x) = d\,\mathrm{diag}\,(x_1, \ldots, x_m)$, $d > 0$, and Neumann boundary conditions.

6.4.1 Passivity

Define the complex affinity as $\gamma(x) = Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right)$. Assuming the existence of a classical solution to (6.4.5), as an immediate consequence we obtain the following energy balance

$$\begin{aligned}
\frac{d}{dt}\mathcal{G}(x) &= \left\langle \frac{\partial G}{\partial x}(x), \frac{\partial x}{\partial t}\right\rangle_{L^2_m(M)} = \left\langle \mu(x), \frac{\partial x}{\partial t}\right\rangle_{L^2_m(M)}\\
&= -\left\langle Z^{\mathrm{T}}\mu(x), B\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}(Z^{\mathrm{T}}\mu(x))\right\rangle_{L^2_m(M)}\\
&\quad + \left\langle \mu(x), \mathrm{div}(\mathcal{R}_d(x)\mathrm{grad}\,\mu(x))\right\rangle_{L^2_m(M)}\\
&= -\left\langle \gamma(x), B\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}(\gamma(x))\right\rangle_{L^2_m(M)}\\
&\quad - \left\langle \mathrm{grad}\,\mu(x), \mathcal{R}_d(x)\mathrm{grad}\,\mu(x)\right\rangle_{L^2_m(M)}\\
&\quad + \left\langle \mu(x), \mathcal{R}_d(x)\mathrm{grad}\,\mu(x)\cdot\nu\right\rangle_{L^2_m(\partial M)}.
\end{aligned} \tag{6.4.7}$$

Because the exponential function is strictly increasing the following inequality holds

$$\begin{aligned}\gamma^{\mathrm{T}} B\mathcal{K}B^{\mathrm{T}}\mathrm{Exp}(\gamma) &= \sum_{j=1}^{r} \left(\gamma_{\mathcal{P}_j}(x) - \gamma_{\mathcal{S}_j}(x)\right)\left(\exp\left(\gamma_{\mathcal{P}_j}(x)\right) - \exp\left(\gamma_{\mathcal{S}_j}(x)\right)\right)\kappa_j(x^*) \\ &\geq 0\end{aligned}$$

for $\kappa_j(x^*) > 0$, $j = 1, \ldots, r$, which immediately implies

$$\langle Z^{\mathrm{T}}\mu(x), B\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}(Z^{\mathrm{T}}\mu(x))\rangle_{L^2_m(M)} \geq 0\,.$$

Furthermore, since

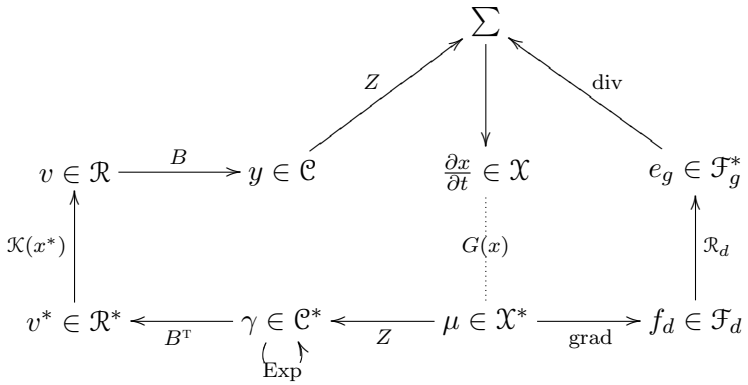
$$\langle \mathrm{grad}\,\mu(x), \mathcal{R}_d(x)\mathrm{grad}\,\mu(x)\rangle_{L^2_m(M)} \geq 0,$$

the *passivity* property holds

$$\frac{d}{dt}\mathcal{G} \leq \langle e_b, f_b\rangle_{L^2_m(\partial M)}\,. \tag{6.4.8}$$

6.4.2 Reaction-Diffusion House

In [101] the authors have offered a geometric interpretation of balanced chemical reaction networks. The geometric interpretation of the reaction-diffusion equations (6.4.5) can be summarized as follows. Denote the dual space of the space of concentrations of chemical species $\mathcal{X} := C^\infty_m(M)$ by $\mathcal{X}^*$. Similarly, denote the dual space of $\mathcal{C} := C^\infty_c(M)$ by $\mathcal{C}^*$, and the dual of the space of reaction rates $\mathcal{R} = C^\infty_r(M)$ by $\mathcal{R}^*$. Define $v^* := B^{\mathrm{T}}\mathrm{Exp}(\gamma)$ and $y := Bv(x)$ at each base point of the spatial domain M. All ingredients of the equation (6.4.5) are then summarized in the following diagram



(6.4.9)

where the effects of the reaction system are expressed on the left-hand side and the contribution of the diffusion on the right-hand side. The concentration vector x and its time-derivative $\frac{\partial x}{\partial t}$ are elements of the linear space $\mathcal{X}$, while the chemical potential vector $\mu \in \mathcal{X}^*$. The state x and the potential μ are related by the Gibbs' function $G(x)$ as $\mu = \frac{\partial G}{\partial x}(x)$. Furthermore, the vector y is in the linear space $\mathcal{C}$, with conjugate vector the complex affinity γ. The duality between μ and γ is given by $\gamma = Z^{\mathrm{T}}\mu$. The gradient of the potential belongs to the space $\mathcal{F}_d := C^\infty_m(M;\mathbb{R}^n)$, whose dual is $\mathcal{F}_d^*$. The relation between y, e_g, and $\frac{\partial x}{\partial t}$ is $\frac{\partial x}{\partial t} = \operatorname{div} e_d + Zy = \operatorname{div} \mathcal{R}_d(f_d) + ZBv$, where $ZB = S$ and $f_d = \operatorname{grad} \mu$. The vector of fluxes v lives in the linear space $\mathcal{R}$, with conjugate vector $v^* := -\big(\mathcal{K}(x^*)\big)^{-1} v \in \mathcal{R}^*$. The added complication in the diagram is the map $\mathrm{Exp} : \mathcal{C}^* \to \mathcal{C}^*$, which introduces a discrepancy between v^* and $\alpha := -B^{\mathrm{T}}\gamma = -S^{\mathrm{T}}\mu$.

6.5 Stability Analysis

> Whereof one cannot speak, thereof one must be silent.
> – Ludwig Wittgenstein, *Tractatus Logico-Philosophicus*

The primary objective of this section is to certify asymptotic stability of the thermodynamic equilibrium for a class of the balanced reaction networks under the influence of diffusion. The notation employed passim this section is the same as in [92, 91, 71], but is briefly described for the reader's convenience.

Let M be a bounded domain in $\mathbb{R}^n$ with $C^{2+\alpha}$ smooth boundary ∂M, where $0 < \alpha \leq 1$. For a Hölder continuous function $g : M \to \mathbb{R}^m$ we denote by $\|.\|_\alpha$, with $0 < \alpha \leq 1$, the Hölder norm

$$\|g\|_\alpha = \sup_{\substack{\xi \neq \bar{\xi} \\ \xi, \bar{\xi} \in M}} \frac{\|g(\xi) - g(\bar{\xi})\|}{\|\xi - \bar{\xi}\|^\alpha}\,.$$

For g in the Banach space $C^{2+\alpha}(M)$ the norm is

$$\|g\|_{2+\alpha} = \|g\|_\infty + \sum_{p=1}^n \left\| \frac{\partial g}{\partial \xi_p} \right\|_\infty + \sum_{p,r=1}^n \left\| \frac{\partial^2 g}{\partial \xi_p \partial \xi_r} \right\|_\infty + \sum_{p,r=1}^n \left\| \frac{\partial^2 g}{\partial \xi_p \partial \xi_r} \right\|_\alpha , \quad (6.5.1)$$

where $\|.\|_\infty$ is the usual sup norm. The first three terms in (6.5.1) constitute the norm of the space $C^2(M)$ and hereafter will be denoted as $\|.\|_2$.

We need a number of technical assumptions to ensure local existence of the solution. Consider the system

$$\begin{aligned} \frac{\partial x}{\partial t}(\xi,t) &= d\Delta x(\xi,t)+g(x), \quad (\xi,t)\in \mathrm{int}M\times(0,T], && (6.5.2)\\ x(\xi,0) &= x_0(\xi)\geq 0, \quad \xi\in M, && (6.5.3)\\ \frac{\partial x}{\partial \nu}(\xi,t) &= 0, \quad (\xi,t)\in \partial M\times(0,T], && (6.5.4) \end{aligned}$$

where d is positive constant and $\mathrm{int}M$ stands for the interior of the domain M.

We consider the following theorem. The first part on local existence is from [2] and the second on global boundedness in $C^{2+\alpha}$ is from [90].

Theorem 6.5.1. *Assume that $d>0$, $x_0(\xi)\in C^{2+\alpha}(M)$ and $\partial x_0/\partial\nu=0$ on ∂M. Assume that $x\mapsto g(x)$ is a locally Lipschitz continuous function. Then there is a $T>0$ such that (6.5.2)-(6.5.4) has a unique local classical solution $(\xi,t)\mapsto x(\xi,t)\in C^2(\mathrm{int}M\times[0,T])\cap C^1(M\times[0,T])$.*

If there is an a priori estimate

$$\|x(\xi,t)\|\leq K\,, \tag{6.5.5}$$

where K is independent of t, then the solution $x(\xi,t)$ exists for all $t>0$ and is bounded in $C^{2+\alpha}(M)$

$$\sup_{t\geq 0}\|x(\xi,t)\|_{2+\alpha}=K_s<\infty\,. \tag{6.5.6}$$

The global boundedness of $(\xi,t)\mapsto x(\xi,t)$ guarantees that the set $\{x(\xi,t)|\ t\geq 0\}$ is relatively compact in $C^2(M)$, see [91]. By definition of a compact set, given a sequence $\{t_k\}$ such that $t_k\to\infty$ as $k\to\infty$, there is $\{\tau_k\}\to\infty$ such that

$$y(\xi)=\lim_{k\to\infty}x(\xi,\tau_k)\ \text{ in }\ C^2(M).$$

The ω-limit set for the system (6.5.2)–(6.5.4) when $T=\infty$ is defined as follows.

Definition 6.5.1. *The ω-limit set of the solution $(\xi,t)\mapsto x(\xi,t)$ is the following set of functions of $\xi\mapsto y(\xi)$:*

$$\omega^+=\left\{y(\xi)\in C^2(M)|\ \lim_{k\to\infty}\|x(\xi,t_k)-y(\xi)\|_2=0 \text{ for some } t_k\to\infty\right\}. \tag{6.5.7}$$

The ω^+ limit set is a nonempty and compact set of $C^2(M)$ if $x(\xi,t)$ is bounded in $C^{2+\alpha}$ (cf. Theorem 1 in [92]).

In order to prove spatial uniformity of the steady state for a class of balanced reaction-diffusion systems, we will need four technical lemmas. The formulations of these well-known lemmas are given in [71, 91, 92, 131].

Lemma 6.5.2. *If the functions* $(\xi,t)\mapsto\phi(\xi,t)$ *and* $(\xi,t)\mapsto\psi(\xi,t)$ *belong to* $C^2(\mathrm{int}M\times(0,T])\cap C^1(M\times[0,T])$ *and satisfy*

$$\begin{aligned}\frac{\partial\phi}{\partial t}\le L(\phi)\quad &\textit{and}\quad \frac{\partial\psi}{\partial t}\ge L(\psi)\quad (\xi,t)\in M\times(0,T]\,,\\ \phi(\xi,0)\le\psi(\xi,0),\quad &\xi\in M\,,\\ \frac{\partial\phi}{\partial\nu}\le\frac{\partial\psi}{\partial\nu}\,,\quad &(\xi,t)\in\partial M\times(0,T]\,,\end{aligned}\tag{6.5.8}$$

where L *is a uniformly elliptic operator, then* $\phi\le\psi$ *in* $M\times[0,T]$.

Lemma 6.5.3. *Assume that the function* $\phi\in C^2(\mathrm{int}M\times(0,T])\cap C^1(M\times[0,T])$ *satisfies*

$$\begin{aligned}\frac{\partial\phi}{\partial t}&=d\Delta\phi,\quad (\xi,t)\in\mathrm{int}M\times(0,\infty)\,,\\ \frac{\partial\phi}{\partial\nu}&=0\quad (\xi,t)\in\partial M\times(0,\infty)\,,\end{aligned}\tag{6.5.9}$$

and that $\phi(\xi,0)\in C^{2+\alpha}(M)$. *Then*

$$\lim_{t\to\infty}\|\phi(\xi,t)-c\|_2=0\,,$$

with

$$c=\frac{1}{|M|}\int_M\phi(\xi,t)\mathrm{d}\xi\,,$$

where $|M|$ *is the volume of* M.

Lemma 6.5.4. *Assume that* $(\xi,t)\mapsto x(\xi,t)$ *and* $(\xi,t)\mapsto y(\xi,t)$ *are solutions of (6.5.2)-(6.5.4) whose initial condition satisfy*

$$\|x(\xi,0)-y(\xi,0)\|\le\rho\ \textit{in}\ M\,.$$

If $g:\mathbb{R}^n\to\mathbb{R}^n$ *satisfies the Lipschitz condition*

$$\|g(z)-g(\bar z)\|\le K\|z-\bar z\|\,,$$

then

$$\|x(\xi,t)-y(\xi,t)\|\le\rho\exp(Kt)\ \textit{in}\ M\times[0,T]\,.$$

Lemma 6.5.5. *Let $(\xi,t)\mapsto G(\xi,t)$ be a bounded function from below satisfying $\partial G/\partial t - d\Delta G \le 0$ in $\mathrm{int}M\times(0,\infty)$ and $\partial G/\partial\nu = 0$ on $\partial M\times(0,\infty)$. Then the function*

$$h(t) = \frac{1}{|M|}\int_M G(\xi,t)\mathrm{d}\xi$$

is decreasing, and $\lim_{t\to\infty} G(\xi,t) = a$ uniformly in $C^2(M)$.

Constant diffusion system. The reaction-diffusion system we consider is

$$\begin{aligned}
\frac{\partial x}{\partial t}(\xi,t) &= d\Delta x(\xi,t) + f(x), \quad (\xi,t)\in M\times(0,T], && (6.5.10)\\
x(\xi,0) &= x_0(\xi) > 0, \quad \xi\in M, && (6.5.11)\\
\frac{\partial x}{\partial \nu}(\xi,t) &= 0, \quad (\xi,t)\in \partial M\times(0,T], && (6.5.12)
\end{aligned}$$

where T may be ∞, f is given as the right-hand side of (6.2.7), $x_0(\xi)\in C^{2+\alpha}(M)$ and $\partial x_0/\partial\nu = 0$ on ∂M. We write $x = (x_1,\dots,x_m)^{\mathrm{T}}$ for the vector of m concentrations $x_i = x_i(\xi,t)$, $i = 1,\dots,m$. It is clear that we assume that all diffusion coefficients d_i of the standard diagonal diffusion matrix are constant and *equal* to $d > 0$.

Theorem 6.5.6. *For the system (6.5.10)–(6.5.12) there is an a priori estimate of the type (6.5.5), hence $(\xi,t)\mapsto x(\xi,t)$ exists globally for $t\ge 0$. Furthermore, the set ω^+ consists of constant functions only. This means that if $c\in\omega^+$, then $c\in\bar{\mathbb{R}}^m_+$ and there exists a sequence $\{t_k\}$ such that*

$$\lim_{k\to\infty}\|x(\xi,t_k) - c\|_2 = 0.$$

Proof. Consider $G(x) = x^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right) + (x^* - x)^{\mathrm{T}}\mathbf{1}_m$, where $(\xi,t)\mapsto x(\xi,t)$ is a solution of the reaction-diffusion system (6.5.10)–(6.5.12). Mildly abusing the notation, we will also denote $G(x)$ by $G(\xi,t)$, in order to avoid introducing a new symbol.

Firstly, we show that

$$\frac{\partial G}{\partial t} - d\Delta G \le 0 \ \text{ in } \ \mathrm{int}M\times(0,T].$$

The time derivative of G along the trajectory of (6.5.10)–(6.5.12) is

$$\begin{aligned}
\frac{\partial G}{\partial t} &= \frac{\partial^{\mathrm{T}} G}{\partial x}\left(f(x) + d\Delta x\right)\\
&= \mathrm{Ln}\left(\frac{x}{x^*}\right)^{\mathrm{T}}\left(-ZB\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right)\right) + d\Delta x\right).
\end{aligned}$$

We compute $\nabla G = \frac{\partial^{\mathrm{T}} G}{\partial x} \nabla x$, and then obtain

$$\Delta G = \left(\frac{1}{x}\right)^{\mathrm{T}} |\nabla x|^2 + \mathrm{Ln}\left(\frac{x}{x^*}\right)^{\mathrm{T}} \Delta x\,.$$

We have

$$\begin{aligned}
&\frac{\partial G}{\partial t} - d\Delta G \\
&\quad = -\mathrm{Ln}\left(\frac{x}{x^*}\right)^{\mathrm{T}} ZB\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x}{x^*}\right)\right) - d\left(\frac{1}{x}\right)^{\mathrm{T}} |\nabla x|^2 \\
&\quad = -\gamma^{\mathrm{T}}(x)B\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}(\gamma(x)) - d\sum_{i=1}^{m} \frac{|\nabla x_i|^2}{x_i} \\
&\quad = -\sum_{j=1}^{r} \left(\gamma_{\mathcal{P}_j}(x) - \gamma_{\mathcal{S}_j}(x)\right)\left(\exp\left(\gamma_{\mathcal{P}_j}(x)\right) - \exp\left(\gamma_{\mathcal{S}_j}(x)\right)\right)\kappa_j(x^*) \\
&\qquad - d\sum_{i=1}^{m} \frac{|\nabla x_i|^2}{x_i} \le 0\,.
\end{aligned}$$

Since $\xi \mapsto G(\xi, 0)$ is continuous in M, there is a constant K_G such that

$$\max_{\xi \in M} G(\xi, 0) \le K_G\,.$$

The zero-flux boundary condition on x implies

$$\begin{aligned}
\frac{\partial G}{\partial \nu} &= \left(\frac{\partial^{\mathrm{T}} G}{\partial x}\nabla x\right)\cdot \nu = \left(\mathrm{Ln}\left(\frac{x}{x^*}\right)^{\mathrm{T}} \nabla x\right)\cdot \nu \\
&= \mathrm{Ln}\left(\frac{x}{x^*}\right)^{\mathrm{T}} (\nabla x \cdot \nu) = 0\,.
\end{aligned}$$

In summary, the following holds

$$\begin{aligned}
\frac{\partial G}{\partial t} - d\Delta G \le 0, &\quad (\xi, t) \in \mathrm{int} M \times (0, T], \\
G(\xi, 0) \le K_G,\ \xi \in M, & \\
\frac{\partial G}{\partial \nu} = 0, &\quad (\xi, t) \in \partial M \times (0, T]\,.
\end{aligned}$$

Applying Lemma 6.5.2 to $\phi := G(\xi, t)$ and $\psi := K_G$ in $M \times [0, T]$, it follows that $G(\xi, t) \le K_G$. Thus $0 < x_i(\xi, t) \le \delta$ in $M \times [0, T]$, since $G(x) \to \infty$ as $\|x\| \to \infty$. From the theory of strict positivity of solutions of mass action

kinetics [72], we know that if $x_0(\xi) > 0$, then $x(\xi,t) > 0$ for all $(\xi,t) \in M \times [0,T]$. Therefore by Theorem 6.5.1 *global boundedness* of x in the $C^{2+\alpha}$ norm follows.

Let ω^+ be the ω-limit set of the solution x. Following the proof of Theorem 2 in [91] we will show that if $\bar{y} \in \omega^+$, then $\bar{y} = \text{const}$.

Let $\bar{y}$ be an arbitrary element of ω^+, that is

$$\bar{y}(\xi) = \lim_{k\to\infty} x(\xi, t_k) \ \text{ in } \ C^2(M).$$

By $(\xi,t) \mapsto y(\xi,t)$ we denote the solution to (6.5.10)–(6.5.12) with an initial condition $y(\xi,0) = \bar{y}(\xi)$.

Set $H(\xi,t) = G(y(\xi,t))$ along the solution y. Because the function f is polynomial, it is locally Lipshitz, and since x lies in a bounded set $\{x \in R^m_+ : G(x) \le K_G\}$, there is K such that $\|f(x) - f(y)\| \le K\|x - y\|$. Then, by Lemma 6.5.4, the following estimate holds

$$\|x(\xi, t+t_k) - y(\xi,t)\| \le \|x(\xi,t_k) - \bar{y}(\xi)\| \exp(Kt)\,. \tag{6.5.13}$$

The last inequality implies that $x(\xi, t+t_k) \to y(\xi,t)$ and $G(\xi,t+t_k) \to H(\xi,t)$ uniformly in ξ as $k \to \infty$.

By Lemma 6.5.5, $\lim_{t\to\infty} G(x(\xi, t+t_k)) = \text{const.}$ uniformly in ξ, hence $H(\xi,t) = \text{const.}$ for all ξ and t.

Furthermore, we have

$$\begin{aligned}\frac{\partial H}{\partial t} &- d\Delta H \\ &= -\sum_{j=1}^{r} \left(\gamma_{\mathcal{P}_j}(y) - \gamma_{\mathcal{S}_j}(y)\right)\left(\exp\left(\gamma_{\mathcal{P}_j}(y)\right) - \exp\left(\gamma_{\mathcal{S}_j}(y)\right)\right)\kappa_j(y^*) \\ &\quad - d\sum_{i=1}^{m} \frac{|\nabla y_i|^2}{y_i} \le 0\,.\end{aligned}$$

On the other hand, $\partial H/\partial t = d\Delta H = 0$. Therefore, $\nabla y = 0$. This shows that $y(\xi,t)$ and in particular $y(\xi) = y(\xi,0)$ are independent of ξ. This means that $y = y(t)$ is a solution of the balanced reaction system $\partial y/\partial t = f(y)$. Finally, $\bar{y} = y(\xi,0) = \text{const.}$, which concludes the proof. □

6.5.1 Hypothesis on Stability

> You will reply that reality hasn't the slightest need to be of interest. And I'll answer you that reality may avoid the obligation to be interesting, but that hypothesis may not.
>
> – Jorge Luis Borges, *Death and the Compass*

Consider the reaction-diffusion system (6.4.5), when $R_d(x) > r_d I_m$, $r_d > 0$, with Neumann boundary conditions, $f_b = \text{grad}\mu(x) \cdot \nu = 0$. We have seen that when $D = \text{diag}\left(\frac{1}{x_1}, \ldots, \frac{1}{x_m}\right) R_d(x) = dI_m$, $d > 0$, an a priori bound of x can be derived directly from a differential inequality for the Lyapunov function. For the general case when D is positive-definite, the procedure presented in the previous section *does not* yield a palpable result regarding the boundedness of the solution. Instead, in this section, we *hypothesize* the boundedness of x and at least C^1 smoothness.

As previously introduced, let $G(x) = x^{\mathrm{T}}\text{Ln}\left(\frac{x}{x^*}\right) + (x^* - x)^{\mathrm{T}}\,\mathbf{1}_m$ and $\mathcal{G}(x) = \int_M G(x)\mathrm{d}\xi$. Since G is proper, $\mathcal{G}(x) \geq 0$.

After imposing the boundary conditions $\text{grad}x \cdot \nu = 0$ on ∂M, the time derivative of $\mathcal{G}$ given in (6.4.7) is

$$\begin{aligned}\frac{d}{dt}\mathcal{G}(x) = &- \langle \gamma(x), B\mathcal{K}(x^*)B^{\mathrm{T}}\text{Exp}(\gamma(x))\rangle_{L^2_m(M)} \\ &- \langle \text{grad}\,\mu(x), R_d(x)\text{grad}\,\mu(x)\rangle_{L^2_m(M)}\,.\end{aligned} \tag{6.5.14}$$

Assuming the validity of the *global persistency conjecture*, we have that $\langle \gamma(x), B\mathcal{K}(x^*)B^{\mathrm{T}}\text{Exp}(\gamma(x))\rangle_{L^2_m(M)} = 0$ if and only if $x \in \mathcal{E}$. Because $R_d(x)$ is positive-definite matrix for all x,

$$\begin{aligned}- \langle \text{grad}\,\mu(x), R_d(x)\text{grad}\,\mu(x)\rangle_{L^2_m(M)} &\leq -r_d \langle \text{grad}\,\mu(x), \text{grad}\,\mu(x)\rangle_{L^2_m(M)} \\ &= -r_d \|\text{grad}\,\mu(x)\|^2_{L^2_m(M)} \\ &= 0\end{aligned}$$

if and only if $\|\text{grad}\,\mu(x)\|_{L^2_m(M)} = 0$. Since $\mu = \text{Ln}\left(\frac{x}{x^*}\right)$, the last condition means $\|\text{grad}\,x\|_{L^2_m(M)} = 0$ on M.

Together, the conditions $x \in \mathcal{E}$ and $\|\text{grad}\,\mu(x)\|_{L^2_m(M)} = 0$ on M imply that $\frac{d}{dt}\mathcal{G}(x) = 0$ if and only if $x(\xi) \in \mathcal{E}$ uniformly in ξ on M. By the Krasovskii-LaSalle invariance principle for infinite-dimensional systems [43, 44], it follows that $x \in \mathcal{E}$ is asymptotically stable in L_2 sense.

Conjecture 6.5.7. *The reaction-diffusion system (6.4.5), when $R_d(x) > r_d I_m$, $r_d > 0$, with Neumann boundary conditions, $f_b = \text{grad}\mu(x) \cdot \nu = 0$,* does not *generate spatially nonuniform steady state.*

This speculation about the inability of system (6.4.5) to generate spatial patterns obviously has significant biochemical consequences and thus deserves a proper mathematical treatment. We cease our analysis of the spatially continuous models and for the rest of the chapter focus our attention on structured discretization of reaction-diffusion systems.

6.6 Structure-Preserving Discretization

A single species system. Firstly, let us consider single component reaction-diffusion system

$$\begin{aligned} \frac{\partial x}{\partial t} &= *\mathrm{d} * (D(x)\,\mathrm{d}\,x) + g(x) \\ e_b &= \mathrm{tr}\, x \\ f_b &= \mathrm{tr}\,(*\mathrm{d}\, x)\,, \end{aligned} \tag{6.6.1}$$

where $x, g, D \in \Omega^0(M)$, $D(x) > 0$ for all x, and $e_b \in \Omega^0(M)$ and $f_b \in \Omega^{n-1}(M)$.

Let K be a homological simplicial complex obtained by triangulation of the manifold M. Assume that K is well-centered, its circumcentric dual is $\star K = \star_{\mathrm{i}} K \times \star_{\mathrm{b}} K$. A discrete analogue of (6.6.1) is

$$\begin{aligned} \frac{\partial x}{\partial t} &= (*_0)^{-1} \left(\mathbf{d}_{\mathrm{i}}^{n-1} *_1 D_d(x) \mathbf{d}^0 x + \mathbf{d}_{\mathrm{b}}^{n-1} \hat{f}_b \right) + g(x) \\ e_b &= \mathbf{tr}^0\, x, \end{aligned} \tag{6.6.2}$$

where the state x now lives on the zero-skeleton of K, that is, $x \in \Omega_d^0(K)$, the input $\hat{f}_b \in \Omega_d^{n-1}(\star_{\mathrm{b}} K)$, and the output $e_b \in \Omega_d^0(\partial K)$. The positive-definite diffusion matrix is $x \mapsto D_d(x) \in \mathbb{R}^{N_e \times N_e}$, with $N_e = \dim \Omega_d^1(K)$, while the operators $*_0$, $*_1$, $\mathbf{d}^0$, $\mathbf{d}_{\mathrm{i}}^{n-1}$, $\mathbf{d}_{\mathrm{b}}^{n-1}$, and $\mathbf{tr}^0$ have been defined in Chapter 4. The operator $\mathbf{d}^0 : \Omega(K) \to \Omega^1(K)$ is nothing but the transpose of the incidence matrix of the primal skeleton (from the primal edges to the primal vertices). Furthermore, $\mathbf{d}^0 = -\left(\mathbf{d}_{\mathrm{i}}^{n-1}\right)^{\mathrm{T}}$ and $\mathbf{d}_{\mathrm{b}}^{n-1} = \left(\mathbf{tr}^0\right)^{\mathrm{T}}$. The discrete Hodge operator $*_1 : \Omega^1(K) \to \Omega^{n-1}(\star_{\mathrm{i}} K)$ is a diagonal matrix with the k-th entry being equal $|\star_{\mathrm{i}} \sigma_k^1|/|\sigma_k^1|$, where σ_k^1 is the primal edge with the dual $\star_{\mathrm{i}} \sigma_k^1$. The matrix $*_0$ is a diagonal matrix whose k-th element is $|\star_{\mathrm{i}} \sigma_k^0|/|\sigma_k^0|$.

Remark 6.6.1. *In fact, the model (6.6.2) slightly, but crucially, differs from the standard compartmental model on graphs, where the matrix* $(*_0)^{-1}$ *does not appear [6]. This implies that in the standard graph model* $*_0 = I_N$, $N =$

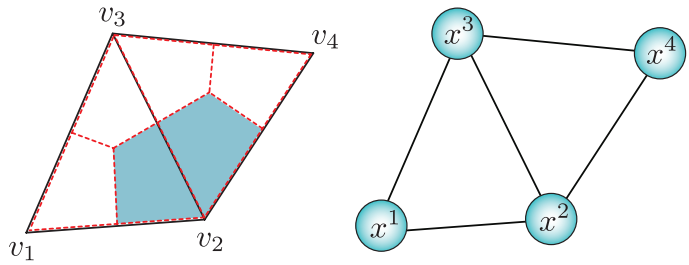


Figure 6.2: A simplicial complex K consisting of two triangles. The dual edges introduced by the circumcentric subdivision are shown dotted. The state vector $x^j = \left(x_1^j, \ldots, x_m^j\right)^{\mathrm{T}}$ is associated to the vertex v_j for each $j \in \{1, \ldots, N\}$. The number of compartments for this example is $N = 4$. The shaded region, the dual cell $*_{\mathrm{i}} v_2$ of the vertex v_2, represents the compartment with the state x^2.

$\dim \Omega_d^0(K)$, *that is,* $|\star_{\mathrm{i}}\, \sigma_k^0| = 1$ *for all* $k = 1, \ldots, N$, *meaning that all the compartments are of* equal *volume. This fact does not surprise, since the graph formulation* does not *capture the* geometric *content of the underlying model.*

Multicomponent system. Let us now consider the reaction-diffusion system with m components (cf. (6.4.5)). To each node of the primal mesh we associate reaction dynamics. That is, to a node σ_j^0 we associate the state $x^j \in \mathbb{R}_+^m$. The geometric dual of σ_j^0, $\star_{\mathrm{i}}\sigma_j^0$, is the dual volume cell which represents the j-th compartment (see Figure 6.2). The number of the compartments is $N = \dim \Omega_d^0(K) = \dim \Omega_d^n(\star_{\mathrm{i}} K)$. The compartments interact with each other through the diffusion modeled as follows.

By X denote the concatenated vector

$$X = \left(\left(x^1\right)^{\mathrm{T}}, \ldots, \left(x^N\right)^{\mathrm{T}}\right)^{\mathrm{T}}, \tag{6.6.3}$$

where $x^j \in \mathbb{R}_+^m$, and let

$$F(X) = \left(f\left(x^1\right)^{\mathrm{T}}, \ldots, f\left(x^N\right)^{\mathrm{T}}\right)^{\mathrm{T}} \tag{6.6.4}$$

be the vector field which describes the reaction dynamics of all compartments, with $f(x^j) = -Z\, B\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x^j}{x^*}\right)\right)$, $j = 1, \ldots, N$, as in (6.4.5).

The ***open compartmental model*** of the reaction-diffusion system (6.4.5) is given by

$$\begin{aligned}\dot{X} = &-\left((*_0)^{-1}\otimes I_m\right)\Big(\left(\mathbf{d}\otimes I_m\right)^{\mathrm{T}}(*_1\otimes I_m)\,R_d(X)\,(\mathbf{d}\otimes I_m)\,\frac{X}{X^*}\\ &\qquad -(\mathbf{tr}\otimes I_m)^{\mathrm{T}}\,\hat{f}_b\Big)+F(X)\\ e_b = &\,(\mathbf{tr}\otimes I_m)\,\frac{X}{X^*}\,,\end{aligned}\tag{6.6.5}$$

where $\otimes$ represents the Kronecker product, I_m is the identity matrix of dimension $m\times m$, $R_d(X)\geq \alpha I_{mN_e}$, $\alpha>0$, and N_e is the number of edges of the primal mesh. Note that we have used $\mathbf{d}$ to denote $\mathbf{d}^0=-\left(\mathbf{d}_{\mathrm{i}}^{n-1}\right)^{\mathrm{T}}$ and $\frac{X}{X^*}=\left(\left(\frac{x^1}{x^*}\right)^{\mathrm{T}},\left(\frac{x^2}{x^*}\right)^{\mathrm{T}},\ldots,\left(\frac{x^N}{x^*}\right)^{\mathrm{T}}\right)^{\mathrm{T}}$.

The total energy of the system, the sum of energies of all compartments, is

$$G_d(X)=\sum_{j=1}^{N}G_j(x^j)V_{\sigma_j^0}\,,$$

where σ_j^0 is the vertex corresponding to the state x^j and $V_{\sigma_j^0}$ is the n-dimensional support volume obtained by taking the convex hull of the simplex σ_j^0 and and its dual cell $\star_{\mathrm{i}}\sigma_j^0$. Since $V_{\sigma_j^0}=|\sigma_j^0||\star_{\mathrm{i}}\,\sigma_j^0|=|\star_{\mathrm{i}}\,\sigma_j^0|$, $j=1,\ldots,N$, the total energy can be written as

$$G_d(X)=\sum_{j=1}^{N}G_j(x^j)|\star_{\mathrm{i}}\,\sigma_j^0|=(G_1,\ldots,G_N)*_0\mathbf{1}_N\,,\tag{6.6.6}$$

where G_j is the Gibb's energy of the j-th compartment given by (6.2.9). The distributed chemical potential as the gradient of (6.6.6) is given as

$$\frac{\partial G_d}{\partial X}=\begin{pmatrix}\frac{\partial G_1}{\partial x^1}|\star_{\mathrm{i}}\,\sigma_1^0|\\ \vdots\\ \frac{\partial G_N}{\partial x^N}|\star_{\mathrm{i}}\,\sigma_N^0|\end{pmatrix}=(*_0\otimes I_m)\,\mathrm{Ln}\left(\frac{X}{X^*}\right).\tag{6.6.7}$$

Compartmental model. Imposing the zero-flux boundary condition, $\hat{f}_b=0$, leads to the closed compartmental model

$$\dot{X}=-\left((*_0)^{-1}\otimes I_m\right)\left(\mathbf{d}\otimes I_m\right)^{\mathrm{T}}(*_1\otimes I_m)\,R_d(X)\,(\mathbf{d}\otimes I_m)\,\frac{X}{X^*}+F(X),\tag{6.6.8}$$

with a positive initial condition $X(0) = X_0 \in \mathbb{R}^{mN}_+$.

A simple but crucial observation is that $F^*_k(X) \geq 0$ when $X_k = 0$ for any $k = 1, \ldots, mN$ and $X \in \bar{\mathbb{R}}^{mN}_+$. We have

$$F^*_k(X) = \underbrace{- Z^i B\mathcal{K}(x^*)B^{\mathrm{T}}\mathrm{Exp}\left(Z^{\mathrm{T}}\mathrm{Ln}\left(\frac{x^j}{x^*}\right)\right)}_{\varsigma^{ij}_R}$$
$$\underbrace{- |\star_{\mathrm{i}}\, \sigma^0_j|^{-1} \left(\mathbf{d}\otimes I_m\right)^{\mathrm{T}}_k (*_1 \otimes I_m)\, R_d(X)\, (\mathbf{d}\otimes I_m)\, \frac{X}{X^*}}_{\varsigma^{ij}_D},$$

where $k = ((j-1)m + i)$ and $X_k = x^j_i$, while Z^i is the i-th row vector of Z and $(\mathbf{d}\otimes I_m)^{\mathrm{T}}_k$ is the k-th column of $(\mathbf{d}\otimes I_m)$.

When $X_k = x^j_i = 0$, the terms corresponding to the positive i-th diagonal element of the weighted Laplacian matrix $B\mathcal{K}(x^*)B^{\mathrm{T}}$ are all zero, while there is at least one term corresponding to a non-zero, and therefore strictly negative, off-diagonal element of $B\mathcal{K}(x^*)B^{\mathrm{T}}$. This implies that $\varsigma^{ij}_R \leq 0$. Similarly, the matrix $(*_1 \otimes I_m)\, R_d(X)$ is a diagonal strictly positive definite matrix, thus the terms corresponding to the positive $((j-1)m+i)$-th diagonal element of the augmented Laplacian matrix $(\mathbf{d}\otimes I_m)^{\mathrm{T}}(*_1\otimes I_m)\, R_d(X)\, (\mathbf{d}\otimes I_m)$ are all zero, while there is at least one off-diagonal negative element. Thus, $\varsigma^{ij}_D \leq 0$, and therefore $F^*(X) \geq 0$ when $X_k = 0$.

Lemma 6.6.1. *Suppose that $X : [0, t^*] \to \bar{\mathbb{R}}^{mN}_+$ is any solution of (6.6.8). Then for any $k = 1, \ldots, mN$:*

$$X_k(0) > 0 \quad \Rightarrow \quad X_k(t^*) > 0.$$

Proof. The proof is a repetition of the arguments given in [118], Lemma 7.1, for a different class of systems.

Suppose that k is so that $X_k(0) > 0$. Let $\Phi : \mathbb{R}^2 \to \mathbb{R}$ be the function which for $t \in [0, t^*]$ and $y \in \mathbb{R}$ coincides with

$$\Phi(t, y) := F^*_k\big(X_1(t), \ldots X_{k-1}(t), y, X_{k+1}(t), \ldots, X_{mN}(t)\big)$$

and has $\Phi(t, y) = \Phi(0, y)$ for $t < 0$ and $\Phi(t, y) = \Phi(t^*, y)$ for $t > t^*$. Since $F^*_k(X) \geq 0$ when $X_k = 0$, $\Phi(t, 0) \geq 0$ for all t. For $t \in [0, t^*]$, the scalar function $y(t) := X_k(t)$ satisfies $\dot{y}(t) = \Phi(t, y(t))$. We need to prove that y never vanishes. To this end, let

$$\Psi(t, p) := \Phi(t, p) - \Phi(t, 0),$$

and let

$$\dot{z}(t) = \Psi(t, z(t)) \quad \text{with} \quad z(0) = y(0).$$

Because Ψ is locally Lipschitz and 0 is an equilibrium of $\dot{z} = \Phi(t, z)$, $z(t) > 0$ for all t. Furthermore, $\dot{z} = \Psi(t, z) \leq \Phi(t, z)$ for all t, and thus by comparison $z(t) \leq y(t)$.

Since $y(t^*)$ is well-defined, $z(t)$ remains bounded, and thus is defined for $t = t^*$. Hence, $y(t^*) \geq z(t^*) > 0$. □

Corollary 6.6.2. *For the system (6.6.8) the positive orthant $\mathbb{R}^{mN}_+$ is forward invariant.*

Jus like in the case of the system (6.2.7), in order to exclude the existence of possible boundary equilibria, we shall assume the global persistency property.

Conjecture 6.6.3. *Given $X_0 \in \mathbb{R}^{mN}_+$, all the trajectories $t \mapsto X(t)$ of (6.6.8) satisfy:* $\liminf_{t\to\infty} X(t) > 0$.

In the absence of the diffusion terms, the dynamics of the spatially discrete systems are decoupled, and as such coincide with the dynamics of the balanced reaction system (6.2.7). In this scenario all the compartments exhibit asymptotically stable dynamics, but the steady states of the all compartments, in general, are not identical. The following theorem shows that the compartmental model (6.6.8) is asymptotically stable with the spatially uniform steady state.

Theorem 6.6.4. *Consider the compartmental model of balanced mass action reaction network given by (6.6.8). For every initial condition $X(0) \in \mathbb{R}^{mN}_+$, the species concentrations $x^1, x^2, \ldots, x^N$ as $t \to \infty$ converge to $x^1 = x^2 = \cdots = x^N \in \mathcal{E}$.*

Proof. In [101] the authors have shown that G in (6.2.9) satisfies $G(x^*) = 0$ and $G(x) > 0$, $\forall x \neq x^*$, and for every real $c > 0$ the set $\{x \in \bar{\mathbb{R}}^m_+ \mid G(x) \leq c\}$ is compact. This easily can be checked. Let x_i and x^*_i denote the i-th elements of x and x^* respectively. From the strict concavity of the logarithmic function $z - 1 \geq \ln(z)$, $\forall z \in \mathbb{R}_+$, with equality if and only if $z = 1$. Putting $z = \frac{x^*_i}{x_i}$, we have $x^*_i - x_i + x_i \ln\left(\frac{x_i}{x^*_i}\right) \geq 0$, with equality if and only if $x_i = x^*_i$. This implies that $G(x) = \sum_{i=1}^m \left(x^*_i - x_i + x_i \ln\left(\frac{x_i}{x^*_i}\right)\right) \geq 0$, with equality if and only if $x_i = x^*_i, i = 1, \cdots, m$. Thus G has a strict minimum at $x = x^*$ and and $G(x) > 0$, $\forall x \neq x^*$.

The above stated properties of G immediately imply that the function $X \mapsto G_d(X)$ in (6.6.6) satisfies

$$G_d(X^*) = 0, \quad G_d(X) > 0, \quad \forall X \neq X^*, \tag{6.6.9}$$

and is *proper*, i.e., for every real $C > 0$ the set $\{X \in \bar{\mathbb{R}}_+^{mN} \mid G_d(X) \leq C\}$ is compact.

In what follows we will show that $\dot{G}_d(X) = \frac{\partial^{\mathrm{T}} G_d}{\partial X}(X)\dot{X} = \frac{dG_d}{dt}(X)$ satisfies

$$\dot{G}_d(X) \leq 0 \text{ for all } X \in \mathbb{R}_+^{mN}, \tag{6.6.10}$$

and

$$\dot{G}_d(X) = 0 \text{ if and only if } x^1 = x^2 = \cdots = x^N \in \mathcal{E}. \tag{6.6.11}$$

We look for the time derivative of the total energy:

$$\begin{aligned}
\dot{G}_d = \frac{\partial^{\mathrm{T}} G_d}{\partial X}\dot{X} &= \left((*_0 \otimes I_m)\,\mathrm{Ln}\left(\frac{X}{X^*}\right)\right)^{\mathrm{T}} \dot{X} \\
&= -\mathrm{Ln}\left(\frac{X}{X^*}\right)^{\mathrm{T}} (*_0 \otimes I_m)^{\mathrm{T}} \left((*_0)^{-1} \otimes I_m\right) \\
&\qquad \cdot (\mathbf{d} \otimes I_m)^{\mathrm{T}} (*_1 \otimes I_m)\, R_d(X)\, (\mathbf{d} \otimes I_m)\, \frac{X}{X^*} \\
&\qquad + \mathrm{Ln}\left(\frac{X}{X^*}\right)^{\mathrm{T}} (*_0 \otimes I_m)^{\mathrm{T}} F(X).
\end{aligned} \tag{6.6.12}$$

Since $(*_0 \otimes I_m)^{\mathrm{T}} \left((*_0)^{-1} \otimes I_m\right) = I_{mN}$, we have

$$\begin{aligned}
\dot{G}_d &= -\mathrm{Ln}\left(\frac{X}{X^*}\right)^{\mathrm{T}} (\mathbf{d} \otimes I_m)^{\mathrm{T}} (*_1 \otimes I_m)\, R_d(X)\, (\mathbf{d} \otimes I_m)\, \frac{X}{X^*} \\
&\quad + \mathrm{Ln}\left(\frac{X}{X^*}\right)^{\mathrm{T}} (*_0 \otimes I_m)^{\mathrm{T}} F(X) \\
&= -\left((\mathbf{d} \otimes I_m)\,\mathrm{Ln}\left(\frac{X}{X^*}\right)\right)^{\mathrm{T}} (*_1 \otimes I_m)\, R_d(X)\, (\mathbf{d} \otimes I_m)\, \frac{X}{X^*} \\
&\quad + \sum_{i=1}^{N} |\star_{\mathrm{i}}\, \sigma_i^0| \underbrace{\frac{\partial^{\mathrm{T}} G_i}{\partial x^i} f(x^i)}_{\varepsilon_R(x^i)} \\
&= -\underbrace{\left\langle (\mathbf{d} \otimes I_m)\,\mathrm{Ln}\left(\frac{X}{X^*}\right), R_d(X)\, (\mathbf{d} \otimes I_m)\, \frac{X}{X^*} \right\rangle_d}_{\varepsilon_D} \\
&\quad + \sum_{i=1}^{N} |\star_{\mathrm{i}}\, \sigma_i^0| \varepsilon_R(x^i).
\end{aligned} \tag{6.6.13}$$

We compute the expression $\varepsilon_R(x^i)$, along the lines of [101], as

$$\begin{aligned}\varepsilon_R(x^i) &= \tfrac{\partial^{\mathrm{T}} G_i}{\partial x^i} f(x^i) \\ &= -\mu^{\mathrm{T}}(x^i) Z B \mathcal{K}(x^*) B^{\mathrm{T}} \mathrm{Exp}(Z^{\mathrm{T}} \mu(x^i)) \\ &= -\gamma^{\mathrm{T}}(x^i) B \mathcal{K}(x^*) B^{\mathrm{T}} \mathrm{Exp}(\gamma(x^i)) \\ &= \textstyle\sum_{j=1}^{r} \big(\gamma_{\mathcal{S}_j}(x^i) - \gamma_{\mathcal{P}_j}(x^i)\big)\big(\exp\big(\gamma_{\mathcal{P}_j}(x^i)\big) - \exp\big(\gamma_{\mathcal{S}_j}(x^i)\big)\big)\kappa_j(x^*) \\ &\leq 0\,,\end{aligned} \tag{6.6.14}$$

since $\kappa_j(x^*) > 0$ for $j = 1, \ldots, r$, and the exponential function is strictly increasing. The summand in the third line of (6.6.14) is zero only if $\gamma_{\mathcal{S}_j}(x^i) - \gamma_{\mathcal{P}_j}(x^i) = 0$ for every j. This is equivalent to having $B^{\mathrm{T}}\gamma(x) = 0$. Thus, $\varepsilon_R(x^i) = 0$ only if $B^{\mathrm{T}}\gamma = B^{\mathrm{T}} Z^{\mathrm{T}} \mathrm{Ln}\left(\frac{x^i}{x^*}\right) = 0$. It follows that

$$\varepsilon_R(x^i) = 0 \quad \text{if and only if} \quad x^i \in \mathcal{E} \quad \text{for all} \quad i = 1, \ldots, N. \tag{6.6.15}$$

For the contribution of the compartmental diffusion dynamics we have

$$\begin{aligned}\varepsilon_D &= \left\langle (\mathbf{d} \otimes I_m) \frac{\partial G}{\partial X}, R_d(X) (\mathbf{d} \otimes I_m) \frac{X}{X^*} \right\rangle_d \\ &\geq \sum_{k=1}^{N_e} \left(\mathrm{Ln}\left(\frac{x^i}{x^*}\right) - \mathrm{Ln}\left(\frac{x^j}{x^*}\right) \right)^{\mathrm{T}} \alpha |\sigma_k^1| \left(\frac{x^i}{x^*} - \frac{x^j}{x^*} \right) \geq 0\,,\end{aligned}$$

where N_e is the number of edges of the primal mesh, and x^i and x^j are states associated to the nods i and j, and k is the edge between nodes i and j. Because $\ln(\cdot)$ is an increasing function, $\left(\mathrm{Ln}\left(\frac{x^i}{x^*}\right) - \mathrm{Ln}\left(\frac{x^j}{x^*}\right)\right)$ possesses the same sign as $\left(\frac{x^i}{x^*} - \frac{x^j}{x^*}\right)$, and hence $\varepsilon_D \geq 0$. Furthermore,

$$\varepsilon_D = 0 \quad \text{if and only if} \quad x^1 = x^2 = \cdots = x^N. \tag{6.6.16}$$

Now, $\dot{G}_d = 0$ if and only if $\varepsilon_R = 0$ and $\varepsilon_D = 0$. The intersection of the two conditions (6.6.16) and (6.6.15) gives (6.6.11).

Since G_d is proper (in $\bar{\mathbb{R}}_+^{mN}$) and the state trajectory $X(\cdot)$ remains in $\mathbb{R}_+^{mN}$, (6.6.10) implies that $X(\cdot)$ is bounded in $\mathbb{R}_+^{mN}$. Therefore, boundedness of $X(\cdot)$, together with equations (6.6.10) and (6.6.11), by the Krasovskii-LaSalle invariance principle imply that all the species concentrations $x^1, x^2, \ldots, x^N$ converge to an element in $\mathcal{E}$. □

Remark 6.6.2. *Theorem 6.6.4 remains unaltered if we replace the reaction vector field (6.2.7) by any vector function of the form (not corresponding anymore to mass action kinetics)*

$$f(x^j) = -ZB\mathcal{K}_{\text{new}}(x^j, x^*)B^{\text{T}}\Phi\left(Z^{\text{T}}\text{Ln}\left(\frac{x^j}{x^*}\right)\right), \tag{6.6.17}$$

where $\mathcal{K}_{\text{new}}(x^j, x^*) := \text{diag}\big(\kappa_1^{\text{new}}(x^j, x^*), \cdots, \kappa_r^{\text{new}}(x^j, x^*)\big) > 0$ *for all* $x^j \in \mathbb{R}^m_+$ *and* $\Phi : \mathbb{R}^c \to \mathbb{R}^c$ *is a mapping* $\Phi(y_1, \cdots, y_c) = \text{diag}(f_1(y_1), \ldots, f_c(y_c))$, *with the functions* Φ_i, $i = 1, \ldots, c$, *all monotonically increasing.*

In fact, a recent paper [89] *shows that, for instance, Michaelis-Menten kinetics are in the form (6.6.17), where* $K_{\text{new}}(x^j, x^*)$ *is a rational but strictly positive definite matrix.*

6.7 Chemical Example

We illustrate our analysis on a simple chemical reaction model

$$X_1 + X_2 \underset{k_1^{\text{rev}}}{\overset{k_1^{\text{forw}}}{\rightleftharpoons}} X_3 \underset{k_2^{\text{rev}}}{\overset{k_2^{\text{forw}}}{\rightleftharpoons}} X_1 + X_4, \tag{6.7.1}$$

where X_1 is enzyme, X_2 substrate, X_3 intermediate product, and X_4 product. The first (binding) and third (unbinding) steps are reversible. Many reactions in the glycolysis metabolic pathway are of this type.

For instance, *glucose-6-phosphate isomerase* (alternatively known as *phosphoglucose isomerase* or *phosphohexose isomerase*) is an enzyme that catalyzes the conversion of *glucose 6-phosphate* (G6P) into *fructose 6-phosphate* (F6P) in the second step of glycolysis. The change in structure is an isomerization, in which the G6P (X_1) has been converted to F6P (X_4). The freely reversible reaction requires an enzyme X_2, phosphohexose isomerase, to proceed; for more details see, e.g., [12].

The dynamical model of (6.7.1) governed by mass action kinetics is given by

$$\begin{aligned}
\dot{x}_1 &= -k_1^{\text{forw}}x_1x_2 + (k_2^{\text{forw}} + k_1^{\text{rev}})x_3 - k_2^{\text{rev}}x_1x_4 \\
\dot{x}_2 &= -k_1^{\text{forw}}x_1x_2 + k_1^{\text{rev}}x_3 \\
\dot{x}_3 &= k_1^{\text{forw}}x_1x_2 - (k_1^{\text{rev}} + k_2^{\text{forw}})x_3 + k_2^{\text{rev}}x_1x_4 \\
\dot{x}_4 &= k_2^{\text{forw}}x_3 - k_2^{\text{rev}}x_1x_4\,.
\end{aligned} \tag{6.7.2}$$

It easily can be checked that $x_1^* = x_2^* = 1$, $x_3^* = k_1^{\text{forw}}/k_1^{\text{rev}}$, $x_4^* = k_1^{\text{forw}}k_2^{\text{forw}}/(k_1^{\text{rev}}k_2^{\text{rev}})$ is one of the equilibria of the system (6.7.2). The complex stoichiometric matrix Z, the incidence matrix B, and the stoichiometrric matrix S for

the reaction network (6.7.1) are

$$Z = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{pmatrix}, \quad S = ZB = \begin{pmatrix} -1 & 1 \\ -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{pmatrix}.$$

Since $Z_{\mathcal{S}_1} = (1,1,0,0)^{\mathrm{T}}$, $Z_{\mathcal{P}_1} = Z_{\mathcal{S}_2} = (0,0,1,0)^{\mathrm{T}}$, and $Z_{\mathcal{P}_2} = (1,0,0,1)^{\mathrm{T}}$, for the chosen x^*, the diagonal balanced reaction constants calculated according to (6.2.5) are

$$\mathcal{K}(x^*) = \begin{pmatrix} k_1^{\mathrm{forw}} & 0 \\ 0 & \frac{k_1^{\mathrm{forw}} k_2^{\mathrm{forw}}}{k_1^{\mathrm{rev}}} \end{pmatrix}.$$

The system (6.7.2) now can be rewritten into the form (6.2.10), while the dynamics under the influence of diffusion is given by the reaction-diffusion model (6.4.5).

The spatially uniform asymptotic behavior predicted by Theorem 6.6.4 is demonstrated with the simulation in Figure 6.3. The elements of the matrix R_d in the system (6.6.8) given in terms of the standard diffusion matrix D are $R_d := \big(\mathrm{diag}(\frac{1}{x_1^*}, \ldots, \frac{1}{x_m^*})D\big) \otimes I_m$, where in our case $m = 4$.

Eliminating the effects of diffusion leads to a spatially nonuniform steady state as Figure 6.4 illustrates.

6.8 Observations and Outlook

Diffusion as an isolated process is associated with a homogenizing effect that eliminates the gradients of the constituents and eventually leads to uniform spatial state. However, diffusion in combination with reaction dynamics can produce spatially heterogenous patterns, but also drive the system to global instability. An open problem in this context is to characterize the properties of the operator R_d in the case of spatial inhomogeneous steady state.

Control for reaction-diffusion systems in the port-Hamiltonian framework can be understood as the coupling of a reaction-diffusion system to an additional port-Hamiltonian system that plays the role of the controller. This, among others, enables the application of passivity-based techniques in control synthesis for reaction-diffusion systems. Not resisting the temptation of expressing my sentiment, only by having accurate structured discretization can one hope to approach this challenging enterprise.

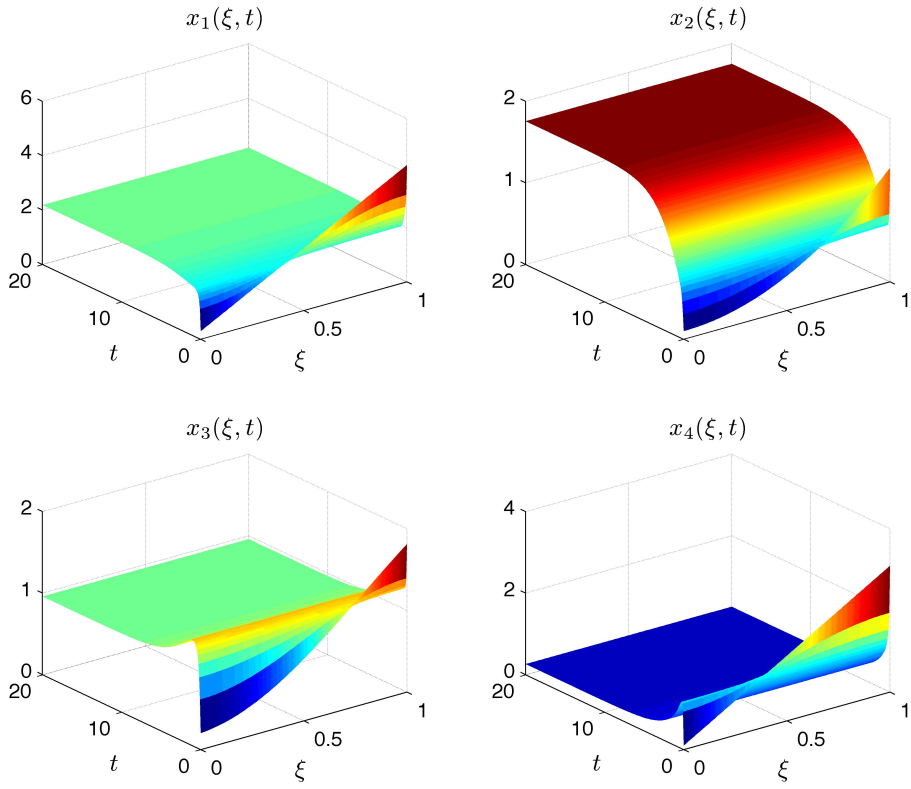


Figure 6.3: Solutions of (6.7.2), in the presence of the diagonal diffusion term $\mathrm{diag}(d_1, d_2, d_3, d_4)\Delta x$, on the one-dimensional spatial domain $M = [0, 1]$ with initial conditions $x_1(\xi, 0) = 4\xi + 0.3$, $x_2(\xi, 0) = 1.3\xi^2 + 0.1$, $x_3(\xi, 0) = 2\sin^2(\xi) + 0.2\xi + 0.2$, $x_4(\xi, 0) = 3\xi + 0.1$, and Neumann boundary conditions. Diffusion coefficients are set to be $d_1 = 0.33$, $d_2 = 0.72$, $d_3 = 0.91$, and $d_4 = 0.67$. The reaction rates are $k_1^{\mathrm{forw}} = 0.1$, $k_1^{\mathrm{rev}} = 0.4$, $k_2^{\mathrm{forw}} = 0.3$, $k_2^{\mathrm{rev}} = 0.5$. Upon the transient phase the system reaches a steady state $x^{**} = x(\xi, \infty) = (2.1856, 1.7557, 0.9602, 0.2638)^{\mathrm{T}}$ uniform in space. Immediately, we verify that x^{**} is a thermodynamical equilibrium, $S^{\mathrm{T}}\mathrm{Ln}(x^{**}) = S^{\mathrm{T}}\mathrm{Ln}(x^*)$. The number of compartments used is $N = 20$.

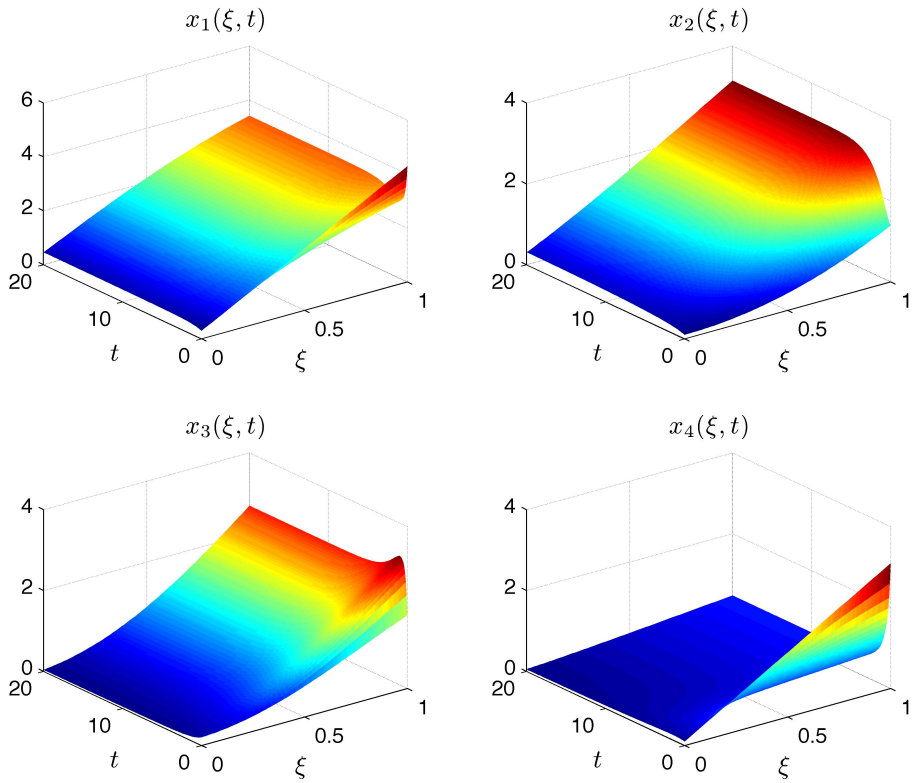


Figure 6.4: Solutions of (6.7.2), in the presence of the diagonal diffusion term $\mathrm{diag}(d_1, d_2, d_3, d_4)\Delta x$, on the one-dimensional spatial domain $M = [0, 1]$ with the initial conditions $x_1(\xi, 0) = 4\xi + 0.3$, $x_2(\xi, 0) = 1.3\xi^2 + 0.1$, $x_3(\xi, 0) = 2\sin^2(\xi) + 0.2\xi + 0.2$, $x_4(\xi, 0) = 3\xi + 0.1$, and Neumann boundary conditions. Diffusion coefficients are set to be $d_1 = d_2 = d_3 = d_4 = 0$. The steady state is not spatially uniform.

7
Conclusion

> Coming to this
> has its rewards: nothing is promised, nothing is taken away.
> We have no heart or saving grace,
> no place to go, no reason to remain.
>
> – Mark Strand, *Coming to This*

In the framework of discrete exterior calculus, I have established a theoretical foundation for formulation of time-continuous spatially-discrete port-Hamiltonian systems. The staple fiber of this approach is the formulation of simplicial Dirac structures as discrete analogues of the Stokes-Dirac structure. These discrete finite-dimensional Dirac structures are the foundation for the definition of open finite-dimensional systems with Hamiltonian dynamics. Such an approach to discretization transfers the essential topological, geometrical, and physical properties from distributed-parameter systems to their finite-dimensional analogues.

The explicit simplicial discretization proposed in Chapter 3 and 4 leads to the standard input-output port-Hamiltonian systems without algebraic constraints. The analysis and the control synthesis for such systems belong to the realm of standard finite-dimensional systems.

Chapter 5 offers a unifying perspective on symmetry reduction of distributed-parameter port-Hamiltonian systems and their discrete analogues on simplicial manifolds of arbitrary finite dimension.

In Chapter 6 I have shown how reaction-diffusion systems can be formulated as port-Hamiltonian systems. Besides offering a clear geometric interpretation, the port-based modeling allows us to look at these systems as interconnected, what simplifies their analysis as has been demonstrated in Section 6.6, where structured discretization of reaction-diffusion systems has led

to finite-dimensional compartmental models.

7.1 What Remains to Be Done, or the Places where I Have Nothing to Contribute to

A number of interesting topics and open questions still need to be addressed. Here I provide a few miscellaneous reflections and some comments on future research.

7.1.1 Numerical Aspects

The discrete exterior calculus employed in this thesis is founded on the idea of a simplicial complex and its circumcentric dual. While for some problems Delaunay triangulation is desirable since it reduces the maximum aspect of the mesh, for others the construction of circumcentric duals might be too expensive (see [105] and references therein). This motivates the development of a discrete calculus on non-simplicial complex meshes, such as a general CW complex [46] or a rectangular scheme. Although the latter might be inappropriate for geometrically complex objects, a potential advantage would be its conceptual simplicity since the circumcentric dual is again a rectangular mesh.

A major challenge from the numerical analysis standpoint is to offer a careful study of the convergence properties of discrete exterior calculus. Furthermore, it would be desirable to have higher-order discrete analogues of the smooth geometric operators. This primarily pertains to deriving higher-accuracy Hodge star operators, which would possibly in return make structure-preserving discretization more competitive even in the domains where structure is put aside. A recent article [8] reports some significant initial results regarding stability of finite element exterior calculus. The abstract theory is applied to linear elliptic partial differential equations with intention to capture the key structure of de Rham cohomology and as such mainly pertains to vanishing boundary constraints. Another related publication [50] extends the framework of [8] to approximate domains. In the future, in the context of [8, 50], it would be interesting to study structure-preserving discretization of port-Hamiltonian systems in the framework of Hilbert complexes.

7.1.2 Open Discretized Systems

The Stokes-Dirac structure has proven to be successful in capturing the essential geometry behind many open systems with Hamiltonian dynamics. The

concept of the Stokes-Dirac structure as presented in the introduction in order to accommodate some port-Hamiltonian systems, such as the ideal isentropic fluid, needs to be augmented [98]. The main idea behind these modifications is again the Stokes theorem. From a structure-preserving discretization point of view, there appears not to be any impediments; nonetheless, in order to discuss these questions in a systematic manner, a unified theory of open infinite-dimensional Hamiltonian systems is needed. The main novelty in discretizing some so formulated general underlying structures might concern their integrability. The simplicial Dirac structures formulated in this thesis are constant Dirac structures and as such they satisfy the usual integrability conditions [23, 25, 29].

An important application of structure-preserving discretization of port-Hamiltonian systems might be in (optimal) control theory, what also prompts a need for time discretization. For closed Hamiltonian systems, it is well-known that asynchronous variational integrators in general cannot preserve the Hamiltonian exactly; however, these integrators, for small time steps, can preserve a nearby Hamiltonian up to exponentially small errors [65, 66, 67, 68, 69]. An important issue in this context is to study the effects these integrators have on passivity (and losslessness) of open dynamical systems.

7.1.3 Poisson Reduction

The idea of Poisson reduction forgoes the analysis conducted in Chapter 5, where the configuration space is a space of differential forms and the symmetry group acts linearly as in (5.3.2). Furthermore, the main idea behind the construction of the Stokes-Dirac structure considered in this thesis applies to a much larger class of systems. How to obtain, for instance, the Lie-Poisson structure of the compressible isentropic fluid with varying boundary condition is an open problem.

7.1.4 Model-Order Reduction

Structure-preserving discretization of distributed-parameter port-Hamiltonian systems leads to high-order port-Hamiltonian systems. This inexorably motivates the search for a structure-preserving model-order reduction, which allows for the replacement of high-order port-Hamiltonian systems with reduced-order models.

A substantial body of work has already been done in this spirit [86, 87, 88, 42], mostly concerning linear models. It would be of considerable importance to look at model-order reduction of the spatially distributed time-continuous

port-Hamiltonian systems obtained in Chapter 4.

7.1.5 Control of Port-Hamiltonian Systems

In Chapter 4 I have been looking at a simple control strategy for the energy shaping of discretized port-Hamiltonian systems. This attempt has only scratched the surface of a very important problem. Since the discretized model assumes a port-Hamiltonian structure, much more elaborate schemes for the control of port-Hamiltonian systems can be applied. A nontrivial problem in this regard would be to design a controller for the discretized model and then test it on the continuous model and obtain the bounds of the discrepancy norm between the two behaviors. Some initial work has already been done in this vein, however, to my knowledge, mostly pertaining to the systems on a one-dimensional spatial domain[1] (see [63, 128, 129, 130] and references quoted there). In higher dimensions, the interconnection of the finite controller and the infinite-dimensional system (plant) would be naturally realized through the interface of the simplicial triangulation of the boundary.

Defining the appropriate discrepancy norms is a subtle task in its own right. The energy norms employed in Section 4.4 seem to be the most natural choice when dealing with port-Hamiltonian systems, but other choices might be even more convenient. Here we are still innocently playing on the sea-shore whilst the great ocean of possibilities lays undiscovered before us[2].

7.1.6 Weak Formulation

The port-Hamiltonian systems formulated on the L_2 de Rham complex in Section 2.3.4 $\big($cf. (2.3.31)$\big)$ are *not* well-posed systems. For instance, take Maxwell's equations as an illustration. Using the tangential component of the electric field intensity on the boundary ∂M as the input and the tangential component of the magnetic field intensity on ∂M as the output, or the other way around, the system (2.3.31) is not well-posed [133]. Introducing the scattering boundary variables in the case of Maxwell's equations leads to a well-posed system [133]. It is not a stretch to expect that a scattering representation of (2.3.31), with a quadratic Hamiltonian density, would be always well-posed, but this remains to be formally proven. How to generically extend

[1] If all the port interconnections were of the punctiform type, as once they have been, the universe would be a much easier place to understand, as Calvino explains it in "All at One Point" in *Cosmicomics*.

[2] Is it possible to paraphrase this giant without feeling like Snoopy?

these results to nonlinear port-Hamiltonian systems is the problem that awaits its solution for quite some time now.

Hilbert spaces are general enough to cover a large class of physical systems, while simultaneously offer a rich toolbox for the analysis of such systems. A natural question arises concerning the *naturality* of the Hilbert-based formulation. The ill-posedness of port-Hamiltonian systems compels me to believe that we should be dealing with more general formulations of open Hamiltonian systems. General Banach spaces, for instance, might offer a more appropriate gadget for the analysis of boundary controlled systems.

7.1.7 Covariant Formulation

It is known that, for instance, Maxwell's equations are also consonant with multisymplectic structures since they can be derived from the Hamiltonian variational principle [1, 67]. The multisymplectic structure behind Maxwell's equations, unlike the Stokes-Dirac structure, is defined, not on a spatial manifold M, but on a spacetime manifold X. Here we need to notice that one could define a Stokes-Dirac type structure on a pseudo-Riemannian, say Lorentzian, manifold. In Lorentzian spacetime, the forms E and B can be combined into a single object, the Faraday 2-form $F = E \wedge \mathrm{d}t + B$. The form F can also be expressed in terms of the electromagnetic potential 1-form A as $F = \mathrm{d}A$. The Hodge star of F is a dual 2-form $G = *F = H \wedge \mathrm{d}t - D$, known as the Maxwell 2-form. The charge density ρ and current density J can be combined into the source 3-form $j = J \wedge \mathrm{d}t - \rho$. A well-known relativistically covariant formulation of Maxwell's equations [1] is: $\mathrm{d}F = 0$ and $\mathrm{d}G = j$.

In order to relate this formulation to the port-Hamiltonian framework, define the following Stokes-Dirac structure on a Lorentzian manifold X by

$$\begin{aligned}\mathcal{D}_{\mathcal{L}} = \big\{ & (f_p, f_q, f_b, e_p, e_q, e_b) \in \\ & \Omega^2(X) \times \Omega^3(X) \times \Omega^2(\partial X) \times \Omega^2(X) \times \Omega^1(X) \times \Omega^1(\partial X) \big| \\ & f_p = -\mathrm{d}e_q \,, f_q = \mathrm{d}e_p \,, e_b = -e_q|_{\partial X} \,, f_b = e_p|_{\partial X} \big\} \,.\end{aligned} \tag{7.1.1}$$

Similar to the proof of Theorem 2.2.1, it is easy to verify that $\mathcal{D}_{\mathcal{L}} = \mathcal{D}_{\mathcal{L}}{}^{\perp}$, with respect to a natural bilinear form. The dynamics of Maxwell's equations can now be imposed by setting $f_p = j$, $f_q = F$, $e_p = A$, and $e_q = G$. Furthermore, since $\mathrm{d}^2 = 0$, it follows that $\mathrm{d}f_p = \mathrm{d}\mathrm{d}e_q = 0$.

A natural choice for discretization of the structure $\mathcal{D}_{\mathcal{L}}$, in the context of discrete exterior calculus, would be on a simplicial 4-complex. This would insure a completely covariant formulation of discrete Maxwell's equations, similar to Regge's formalism for producing simplicial approximations of spacetime

in numerical general relativity [93]. The relativistic effects in most engineering applications are however negligible, hence for these purposes, by choosing a time coordinate, we can split the Lorentzian manifold into $3 + 1$ space, whose discrete analogue is a prismal cell complex. Similar to discretization of multisymplectic structures, this would lead to a certain type of asynchronous variational integrator.

An important and challenging avenue for future work is to make an explicit relation between multisymplectic and Stokes-Dirac structures, and then to compare their discrete analogues.

7.1.8 Structural Aspects of Reaction-Diffusion Systems

In Chapter 6 I have provided a geometric formulation of reaction-diffusion systems with a thermodynamical equilibrium. A model obtained by structure-preserving scheme for the spatial discretization is a compartmental model, which exhibits a striking similarity with consensus dynamics [76, 21]. Exploring this resemblance is a very appealing research direction.

Certifying the spatial uniformity of the steady state for the balanced reaction networks under the influence of diffusion would be a fine thing to hack.

7.2 Coming to This

In conclusion, the discrete exterior calculus approach to discretization preserves a number of important topological and geometrical structures of the the underlying continuous models. In this manner, Dirac structures arising from smooth and discrete models can be treated in a unified framework. The consequences of this are that many of the important results from the continuous geometry can be transferred into the discrete realm and thereby lead to numerically and physically faithful models, which later can be fed to computers and simulate crucial aspects of the physical reality.

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Samenvatting

Dit proefschrift behandelt de structuurbehoudende discretisatie van open verdeelde-parameter systemen met gegeneraliseerde Hamiltonse dynamica. Gebruikmakend van het formalisme van discrete uitwendige differentiaalrekening voer ik simpliciale Diracstructuren in als discrete analogieen van de Stokes-Diracstructuur, en laat ik zien hoe zij een natuurlijk kader bieden om eindigdimensionale poort-Hamiltonse systemen af te leiden die hun oneindigdimensionale tegenhangers nabootsen. Het ruimtelijke domein, in de continue theorie weergegeven door een eindigdimensionale gladde varieteit met rand, wordt vervangen door een homologisch simpliciaal complex en zijn circumcentrische duale. De gladde differentiaalvormen worden in de discrete context vervangen door co-ketens op de primaire en duale complexen, terwijl de discrete uitwendige afgeleide wordt gedefinieerd met behulp van de duale randoperator. Deze benadering door middel van de meetkunde van discrete uitwendige differentiaalrekening maakt het mogelijk om, anders dan het discretiseren van de partiele differentiaalvergelijkingen, eerst de onderliggende Stokes-Diracstructuur te discretiseren en daarna de eindigdimensionale poort-Hamiltonse dynamica hierop te definieren. Op deze manier worden een aantal belangrijke intrinsieke topologische en meetkundige eigenschappen van het systeem behouden. Ik pas deze algemene beschouwingen toe op een aantal fysische voorbeelden, waaronder reactie-diffusie systemen, in welk geval de structuurbehoudende discretisatie het standaard compartimentele model oplevert. Vervolgens laat ik zien hoe op een soortgelijke manier een Poissonsymmetrie reductie van Diracstructuren geassocieerd met oneindig- en eindigdimensionale modellen kan worden uitgevoerd.

Discrete Geometry Approach to Structure-Preserving Discretization of Port-Hamiltonian Systems

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Please mail me comments and corrections.